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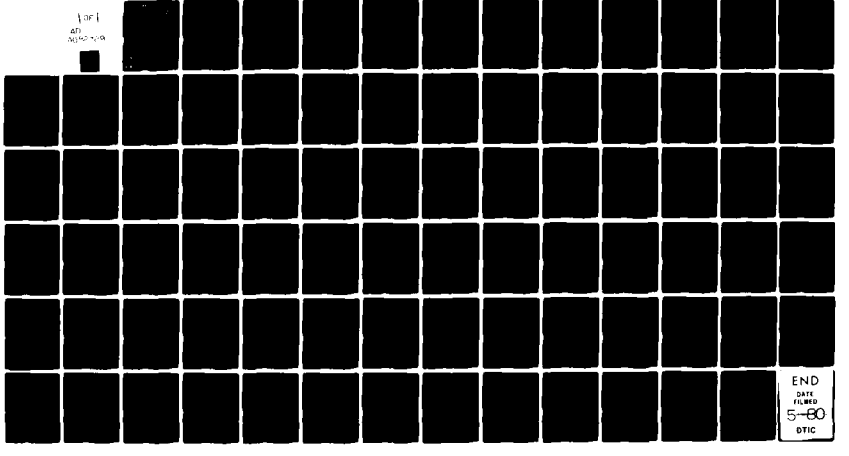

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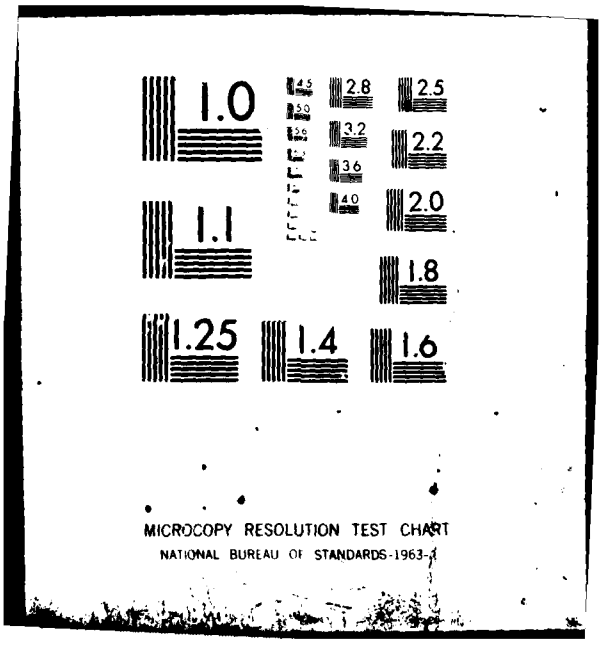
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APPLICATION OF THE METHOD OF LINES TO THE SOLUTION OF ELLIPTIC PARTIAL DIFFERENTIAL EQUATIONS

by
D. J. Jones, J. C. South, Jr.
National Aeronautical Establishment

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(6) # APPLICATION OF THE METHOD OF LINES TO THE SOLUTION OF ELLIPTIC PARTIAL DIFFERENTIAL EQUATIONS

APPLICATION DE LA MÉTHODE DES LIGNES À LA RESOLUTION D'ÉQUATIONS DIFFÉRENTIALES PARTIELLES ELLIPTIQUES

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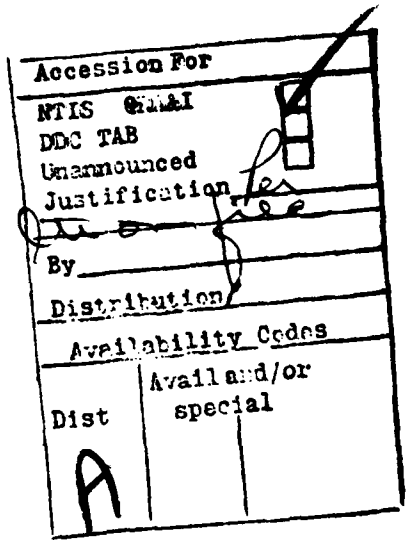
SUMMARY

The method of lines is used in this report for solving one linear, two nonlinear elliptic boundary value problems and a linear eigenvalue problem. An analysis of the stability and convergence is made in the linear cases.

RÉSUMÉ

Dans le présent rapport, on exploite la méthode des lignes pour résoudre un problème linéaire, deux problèmes non linéaires de valeurs elliptiques aux limites et également un problème de valeur propre linéaire. On effectue une analyse de la stabilité et de la convergence dans les situations linéaires.



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APPLICATION OF THE METHOD OF LINES TO THE SOLUTION OF ELLIPTIC PARTIAL DIFFERENTIAL EQUATIONS

CHAPTER 1.0 INTRODUCTION

The method described in this report is known as the method of lines (from here on we refer to the method as MOL) in the Soviet Union, where it has been used for some forty years. The basic feature of the method is that derivatives with respect to one of the independent variables remain continuous, while derivatives with respect to the other independent variables are replaced by finite-difference approximations. For a two-dimensional problem in a rectangle the region could be considered as divided into strips by dividing lines (hence the name) parallel to one of the axes. At each line the derivatives normal to that line would be replaced by finite differences and the other variable left continuous. Thus the system of partial differential equations is replaced by a system of ordinary differential equations. The resulting ordinary differential equations may then be solved, at least in some cases, by analytic methods. For instance Poisson's equation with linear boundary conditions has received much attention, Liskovets (1965) and Leser and Harrison (1966). In the case of more general equations, particularly those of nonlinear type, analytic solutions of the ordinary differential equations may be impossible and the problem must be treated as a two-point boundary-value problem to be solved numerically. This problem may then be solved by either a boundary-value technique such as finite differences or by the shooting method for two-point boundary-value problems. The former technique would be equivalent to solving the original problem by the grid finite-difference method. The shooting method involves estimating unknown conditions at the initial point and integrating the ordinary differential equations across to the end point. The required boundary conditions at the end point can then be satisfied by iterating on the missing initial conditions. Because of the elliptic nature of the partial differential equations this initial-value integration is strictly improper. Indeed it can be shown (Chapter 3) that the ordinary differential equations are inherently unstable. One of the purposes of this paper is to convince the reader that in many physical problems of interest accurate solutions can readily be obtained by MOL even though the problem is incorrectly posed. It is shown that if the region of interest is divided into sufficiently few strips by the dividing lines then accurate solutions can be obtained by using high-order finite-difference approximations. As more and more strips are taken the results may at first improve but they will eventually become meaningless and the iteration technique will not converge to a solution.

The work done in the Soviet Union on MOL has largely been limited to solving linear equations of elliptic (as well as parabolic and hyperbolic) type. A 1965 review paper by Liskovets gives an extensive list of references to provide the mathematical background and development of MOL. These workers have developed analytic solutions of the linear ordinary differential equations for certain cases. Also, solutions of Poisson's equation with linear boundary conditions were obtained in the United States by Leser and Harrison (1966), again using analytic solutions of the ordinary differential equations.

It appears that MOL (and a similar technique called the method of integral relations) was first used in nonlinear problems for the supersonic blunt-body problem which is of interest to aerodynamicists, Belotserkovskii (1965). Klunker, South and Davis (1971) have discussed more recent applications of the method to the solution of equations of elliptic type such as the supersonic blunt-body problem and conical flow problems which are of great importance in aerodynamics. In general the method has received more attention for solving the correctly posed parabolic type of equation. Aktas (1978) gives a recent review of some applications of MOL to parabolic and hyperbolic as well as elliptic problems.

After describing the method of lines in Chapter 2 we then carry out a stability analysis in Chapter 3. Some examples are next discussed in Chapter 4 and, finally, in Chapter 5, we look at solutions to eigenvalue problems.

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CHAPTER 2.0 THE METHOD OF LINES

2.1 A Description of the Method

In order to describe the method we consider the simple case of Poisson's equation

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} = f(x,y) \tag{2.1}$$

to be solved in a rectangle (see Fig. 2.1) subject the following boundary conditions.

$$\psi = 0 \text{ on } x = 0 \tag{2.2}$$

and

$$\psi = \sin\pi x \text{ on } y = b \tag{2.3}$$

Along y = 0 and along x = a the solutions are to be symmetric.

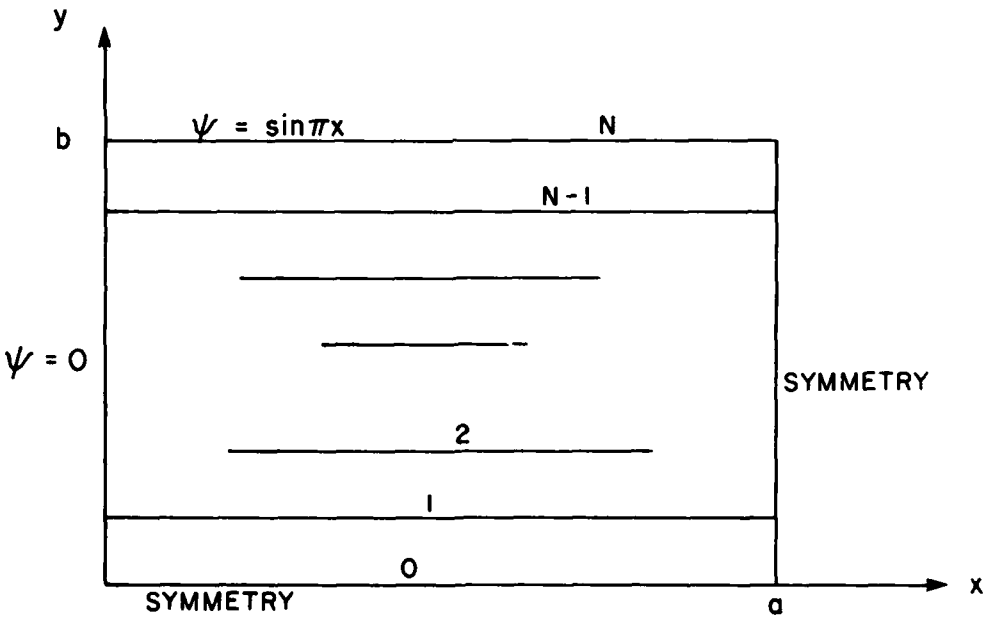

FIG. 2.1 MOL APPLIED TO A RECTANGLE

This simple linear case is sufficiently detailed to describe the principles of the method of lines. More complicated equations and boundary conditions can be solved in the same manner. Minor differences in the treatment of other equations and boundary conditions are seen in the examples of Chapter 4. For example, mixed derivatives and higher order partial differential equations are handled in the Example of Section 4.2.

Other geometries may be treated after transformation as shown later.

We first take equally spaced lines parallel to the x axis and number them (see Fig. 2.1) 0,1,2, . . . N where N is the number of divisions in the region $0 \leqslant y \leqslant b$, thus $h = \frac{b}{N}$.

Next we write the Equation (2.1) as a set of ordinary differential equations. Letting $p = \psi_x$ we have, at each line i (i = 0,1 . . . N-1)

$$\frac{dp_i}{dx} = f(x,y_i) - \frac{\psi_{i+1} - 2\psi_i + \psi_{i-1}}{h^2} \tag{2.4a}$$

$$\frac{d\psi_i}{dx} = p_i \tag{2.4b}$$

since we have approximated ψ_{yy} by the three point difference formula

$$\psi_{yy} = \frac{\psi(x,y+h) - 2\psi(x,y) + \psi(x,y-h)}{h^2} + 0(h^2\psi^{III}) \tag{2.5}$$

At line N we have

$$\psi_N = \sin\pi x \tag{2.6a}$$

while at the image line i = -1 we have

$$\psi_{-1} = \psi_1 \tag{2.6b}$$

The initial and end conditions for the system are

$$\psi_i = 0 \tag{2.7}$$

at x = 0 and

$$p_i = 0 \tag{2.8}$$

at x = a to ensure symmetry of ψ about that point.

The system given by (2.4) is now a system of ordinary differential equations with two point boundary conditions. Thus it can be solved by standard shooting techniques used for solving two point boundary value problems. Some of these methods are given in Keller (1968) in which the

contracting map approach and the variational approach using Newton's method of iteration are described. The latter method is much faster than the former and so is to be recommended. We describe next methods which are similar to the variational approach but which do not set up the variational equations as such. They are thus easier to program and yet still have the advantage of second order convergence. We first discuss Newton's method and then Powell's (1965) method as applied to the shooting technique.

2.2 Newton's Method of Iteration Applied to the Two Point Boundary Value Problem

We first notice that the problem is solved completely provided that we know the initial slopes

$$p_i = F_i$$

($i = 0,1 \ldots N-1$) say at $x = 0$. This is clear since a knowledge of F_i enables us to integrate the Equations (2.4) from $x = 0$ to $x = a$ by standard methods such as Runge Kutta. The present authors normally use Hamming's predictor modifier corrector (PMC) method, see Hamming 1959, with the Runge Kutta starting procedure. The PMC method has a discretization error $0(\delta x^5)$ and requires half as many gradient evaluations as the full Runge Kutta method. On each evaluation of the gradients in (2.4) the boundary conditions (2.6) are used and thus automatically satisfied. Hence integration to $x = a$ (provided round off errors, discretization errors and inherent instability are negligible — see later) is achieved and we recover the boundary condition (2.8). Now, all boundary conditions are satisfied as well as the differential equations and we have a complete solution.

However, since we do not know F_i a priori, we must develop some scheme for improving on a given estimate of F_i. We notice that the only boundary conditions not satisfied after an integration of (2.4) with a given estimate of F_i are the conditions (2.8). The procedure to follow therefore is to drive the values $\dfrac{d\psi_i}{dx}$ at $x = a$ closer to zero by suitably adjusting F_i.

Let

$$\epsilon_i = \frac{d\psi_i}{dx} \tag{2.9}$$

at $x = a$. Then $\Sigma\epsilon_i^2$ can be made smaller by making changes to F_j as indicated by the Newton iteration

$$\sum_{j=0}^{N-1} \frac{\partial \epsilon_i}{\partial F_j} \delta F_j = -\epsilon_i \; (i = 0,1 \ldots N-1) \tag{2.10}$$

The above form requires approximations to the partial derivatives

$$\frac{\partial \epsilon_i}{\partial F_j}$$

To obtain these Keller (1968), amongst others, uses the variational equations. However the present authors have found that it is not necessary to use the variational equations, instead one can write

$$\frac{\partial \epsilon_i}{\partial F_j} \simeq \frac{\epsilon_i(F_0 F_1 \ldots F_j + \Delta F_j \ldots F_{N-1}) - \epsilon_i(F_0 F_1 \ldots F_j \ldots F_{N-1})}{\Delta F_j} \tag{2.11}$$

where ΔF_j is a small value normally taken as $10^{-6}\Delta F_j$ or 10^{-6} if $|\Delta F_j|<1$ (64 bit words with approximately 16 decimal digit accuracy have been used in all our computations). In (2.11) the ϵ_i have been written as functions of $F_0 \ldots F_{N-1}$ since a knowledge of $F_0 \ldots F_{N-1}$ enables us to integrate (2.4) from x = 0 to x = a and so we find the ϵ_i as implicit functions of $F_0 \ldots F_{N-1}$.

Notice that the form (2.11) is exact if ϵ_i is a linear function of $F_0 \ldots F_{N-1}$.

The procedure to find the derivatives

$$\frac{\partial \epsilon_i}{\partial F_j}$$

is therefore to make an integration of (2.4) with the latest estimate $F_0 \ldots F_{N-1}$. Then make successive integrations with F_j changed to $F_j + \Delta F_j$ for j = 0,1 ... N-1 and after each integration substitute into (2.11) to find the required partial derivatives. Having completed these integrations we now substitute (2.11) into (2.10) and find the changes δF_j by standard linear methods such as Gaussian elimination.

The values thus obtained for δF_j can now be used to improve on the last estimate for F_j. This use of δF_j is described below.

2.2.1 The Linear Case

If the differential equations and boundary conditions are linear as in our example then new values of F_j given by

$$F_j = F_j\,(\text{old}) + \delta F_j$$

with δF_j found from (2.10) are the correct values. This follows from the fact that Newton's scheme (2.10) is quadratic in convergence so that if ϵ_i is a linear function of F_j then the correction δF_j is exact. In addition the formula (2.11) is exact for linear systems.

2.2.2 The Nonlinear Case and the Modified Newton Method

It is well known that Newton's method will not, in general, converge if the functions ϵ_i are nonlinear functions of F_j unless the initial estimate is sufficiently near the solution. However it can be shown (see for example Kowalik and Osborne, 1968) that the direction given by (2.10) i.e.

$$\underline{\delta F} = (\delta F_0, \delta F_1, \ldots \delta F_{N-1})$$

is downhill in the sense that $\Sigma\epsilon_i^2$ will decrease by changing F_j such that

$$F_j = F_j\,(\text{old}) + \lambda \delta F_j \tag{2.12}$$

with $\lambda>0$. This feature leads us to the modified Newton procedure whereby λ in (2.12) is chosen such that $\Sigma\epsilon_i^2$ using new values of F_j is less than the previous $\Sigma\epsilon_i^2$ using old values. Thus we select $\lambda = 1$,

compute F_j from (2.12) and hence compute new values of $\Sigma\epsilon_i^2$ by integration as described previously and accept the new values of F_j if they give an improvement to $\Sigma\epsilon_i^2$. If the new values do not yield an improvement we take $\lambda = 1/2$ and repeat the procedure. On successive failures, if they occur, we use $\lambda = 1/4, 1/8 \ldots$ and so on until success is achieved. Once we have a success we then use (2.10) to find a new direction in which to advance. This method has been used successfully by Jones (1973), amongst others.

Some improvement in efficiency can be made to the above modified Newton method and this is now described. Newton's method requires a knowledge of the partial derivatives

$$\frac{\partial \epsilon_i}{\partial F_j}$$

and this determination, from (2.11), may be costly since N integrations of (2.4) are needed. In Newton's method as described above these partial derivatives have to be evaluated at each step given by (2.10). However Newton's method can in some cases be improved on by using the following simplified version (see Collatz (1966) for more details).

Essentially the method consists of using (2.10) repeatedly with values

$$\frac{\partial \epsilon_i}{\partial F_j}$$

unchanged from an earlier step. The simplified version is illustrated in Figure 2.2 for the one unknown F_0. Clearly

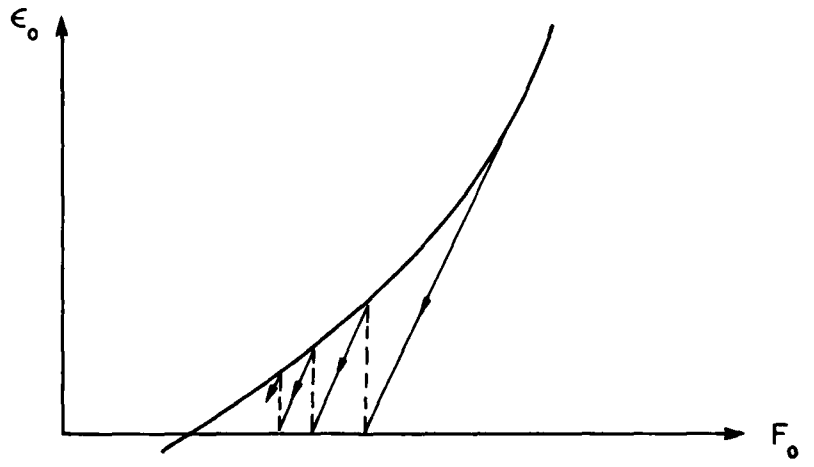

FIG. 2.2 SIMPLIFIED NEWTON METHOD

convergence measured in terms of number of steps is slower. However it has the advantage that the derivatives

$$\frac{\partial \epsilon_i}{\partial F_j}$$

do not have to be evaluated repeatedly nor does the system (2.10) have to be solved completely since the inverse of

$$J = \frac{\partial \underline{\epsilon}}{\partial \underline{F}}$$

can be computed once and stored. South and Klunker (1969) have used this method successfully for conical flow calculations. They find that the method works well if one is sufficiently near the solution. If not one may use several modified Newton steps prior to using the simplified version.

2.3 Powell's Method of Iteration

Powell's method for minimizing a sum of squares of nonlinear functions is given in Powell (1965). The method minimizes

$$\sum_{i=0}^{N-1} \epsilon_i^2$$

with respect to $F_0, F_1 \ldots F_{M-1}$ ($M \leqslant N$), where the N functions ϵ_i are nonlinear functions of the M unknowns F_j. The method is essentially that of least squares minimization in which $\Sigma \epsilon_i^2$ is minimized by making changes to F_j indicated by the direction $\underline{\delta F}$ given by

$$\sum_{j=0}^{M-1} \left\{ \sum_{k=0}^{N-1} \frac{\partial \epsilon_k}{\partial F_i} \frac{\partial \epsilon_k}{\partial F_j} \right\} \delta F_j = - \sum_{k=0}^{N-1} \epsilon_k \frac{\partial \epsilon_k}{\partial F_i} \quad (i = 0 \ldots M-1) \tag{2.13}$$

The step to find new values of $\underline{F} = (F_0, F_1 \ldots F_{M-1})$ is given by

$$\underline{F} = \underline{F}\,(\text{old}) + \lambda \underline{\delta F}$$

in which λ is chosen (by search) such that $\Sigma \epsilon_i^2$ is minimized along the direction $\underline{\delta F}$. During the search along $\underline{\delta F}$ to locate the minimum, functions ϵ_i have to be evaluated at different values of λ; thus one can calculate an approximation, by differences, to the rate of change of ϵ_i along the direction $\underline{\delta F}$ at the new minimum point. Powell shows how these partial derivatives can be used in conjunction with previous values of

$$\frac{\partial \epsilon_k}{\partial F_i}$$

to determine the next step given by (2.13).

In principle the method guarantees convergence since we do not take a step unless $\Sigma\epsilon_i^2$ decreases. In practice the method has been found to fail but only rarely and usually when a poor estimate has been made. Powell's method when it first appeared in 1965 was probably the most efficient method of its day. Other methods which may now be more efficient than Powell's are the spiral method of Jones (1970) and Peckham's (1970) method but these have not been tried on two point boundary value problems.

The advantage of Powell's method over the modified and/or simplified Newton method is firstly that Powell's method is usually more efficient and secondly that fewer "unknowns" can be used to determine the solution. In MOL it may be that the unknown function, in our example

$$\frac{\partial \psi}{\partial x}$$

at x = 0, can be represented in a series expansion, say

$$\frac{\partial \psi}{\partial x} = \sum_{0}^{M-1} F_j \cos jy \qquad (2.14)$$

(M<<N) and in this way the work involved in finding the partial derivatives

$$\frac{\partial \epsilon_i}{\partial F_j}$$

is greatly reduced since now we have to integrate (2.4) only M times to obtain the required partial derivatives. Such a form (2.14) was used in the conical flow calculation by Jones (1968).

Powell's method also has quadratic convergence provided one is sufficiently near the solution and provided $\epsilon_i = 0$ at the minimum. Note that the correct solution is again obtained in one step if the system is linear.

During the preceding discussion the phrase "provided one is sufficiently close to the solution" keeps recurring and indeed it is very important in nonlinear cases to have reasonable estimates of the unknowns particularly to cut down computing costs. In view of the importance we discuss initial estimates in a separate section to follow.

2.4 Initial Estimates

2.4.1 The Linear Case

In the case where the differential equations and boundary conditions are linear the MOL equations can be solved in one step using Newton's or Powell's method **whatever** initial estimate is made.

However the above statement must be viewed with some caution. Although it is true in principle, in practice we clearly have to have an initial estimate which at least allows integration to the end boundary x = a without the solution blowing up. In the authors' experience it is possible to take quite crude estimates such as, at x = 0,

$$\frac{d\psi}{dx} = \frac{\pi y}{b} \tag{2.15}$$

in the example of Section 3.5. Compare this to the exact solution

$$\frac{d\psi}{dx} = \pi \frac{\cosh \pi y}{\cosh \pi b}$$

The motivation behind the choice (2.15) was merely that it satisfied the boundary condition at y = b evaluated at x = 0.

2.4.2 The Nonlinear Case

As has been pointed out it is desirable (and sometimes essential) to have a reasonably good estimate in the nonlinear case. The authors have found that this limitation is not severe for two reasons.

The first reason is that a nonlinear problem can often be made linear by a suitable choice of a parameter in the problem. This linear problem can then be solved with a fairly crude estimate and then the parameter can be varied in discrete steps. To obtain the solution at each value of the parameter a good initial estimate is available by extrapolation from previous results.

The second reason is that a parameter in the problem can often be chosen such that a solution is already known at that value and estimates for each successive values of the parameter are then obtained by extrapolation as above. An example of this is in first setting the angle of incidence to be zero in the conical flow calculations of Section 4.3; this has the effect, for the circular cone, of making the flow axisymmetric and solutions in this case are well known.

Note that such an extrapolation (the authors use quadratic extrapolation as soon as three previous solutions are available) is not restricted by computer storage limitations as it may be in grid techniques. This follows since we have only $0(N)$ unknowns to store rather than $0(N^2)$.

2.5 Termination Procedures

Good termination procedures for nonlinear problems are often difficult to find and some attention should be paid to them. Clearly in the linear case one step is all that is needed and iteration can then cease. Some of the subprograms written for Powell's method terminate when the next change to F_j, δF_j, is less than a certain amount say $|\delta F_j| < \rho$ for some small value of ρ. However in some cases a better criterion might clearly be

$$\left| \frac{\delta F_j}{F_j} \right| < \rho$$

There may be a problem in choosing ρ since too small a value may result in excessive computer time.

The authors have found it better to use a criterion which depends on the size of the residuals of ϵ_i — either

$$\frac{1}{N} \sum_{0}^{N-1} \epsilon_i^2 < \delta$$

or

$$\max_i |\epsilon_i| < \delta$$

for example can be used. In the case of the conical flow calculations of Section 4.3 the choice of residual could be found from physical reasoning and was related to the mass flow into or from the body relative to the total free stream mass flow being less than a certain amount.

A combination of the above criteria together with a preset maximum number of integrations is normally employed.

2.6 Other Systems

In order to describe MOL a simple linear example was discussed. However, the procedure of solution for other systems of equations is identical to that already described, particularly as we have already covered Newton's and Powell's methods for solving nonlinear problems. The user may need to use other finite difference formulas, for example for a first derivative we could write

$$\frac{\partial \psi}{\partial y} = \frac{\psi(x,y+h) - \psi(x,y-h)}{2h} + 0(h^2 \psi^{III}) \tag{2.16}$$

Formulas (2.5) and (2.16), accurate to $0(h^2)$, which use values on 3 adjacent lines, may be used in MOL applications. However a decided improvement can be obtained by using formulas obtained from values on five adjacent lines. These formulas are

$$\frac{\partial \psi}{\partial y} = \frac{4}{3} \frac{\psi(x,y+h) - \psi(x,y-h)}{2h} - \frac{1}{3} \frac{\psi(x,y+2h) - \psi(x,y-2h)}{4h} + 0(h^4 \psi^{V}) \tag{2.17a}$$

and

$$\frac{\partial^2 \psi}{\partial y^2} = \frac{4}{3} \frac{\psi(x,y+h) + \psi(x,y-h) - 2\psi(x,y)}{h^2} - \frac{1}{3} \frac{\psi(x,y+2h) + \psi(x,y-2h) - 2\psi(x,y)}{4h^2} + 0(h^4 \psi^{VI}) \tag{2.17b}$$

The advantages of using the five line schemes (2.17) in place of the three line schemes is shown below. The next section then gives difference formulas of the same accuracy $0(h^4)$ as (2.17) which can be used on the boundary or at the line adjacent to the boundary.

Suppose E represents the exact derivative of a function ψ with respect to y and let A_1 and A_2 represent the approximations given by Equations (2.16) and (2.17a) respectively. Then it can be shown, by looking at the truncation errors, that

$$\epsilon_1 = \left|1 - \frac{A_1}{E}\right| \simeq \frac{\delta y_1^2}{6} \left|\frac{\psi^{III}}{\psi^I}\right|$$

and that

$$\epsilon_2 = \left|1 - \frac{A_2}{E}\right| \simeq \frac{\delta y_2^4}{24} \left|\frac{\psi^V}{\psi^I}\right|$$

where δy_1 and δy_2 are the finite-difference increments. Now we want to find the ratio $\delta y_2 : \delta y_1$ to give the same accuracy in both formulas, i.e., $\epsilon_1 = \epsilon_2 = \epsilon$. For this condition we have

$$\frac{\delta y_2}{\delta y_1} \simeq 0.90 \left|\frac{\psi^{III^2}}{\psi^V \psi^I}\right|^{1/4} \epsilon^{-1/4} \qquad (2.18)$$

The value of $\epsilon^{1/4} \delta y_2 / \delta y_1$ can be calculated from this formula for well-known functions. Its value is approximately 0.90 for sin ny, cos ny and exp(ny), while for log y its value is 0.57. Hence provided the approximate formula (2.18) holds, it can be seen that if ϵ is, say 10^{-4} (0.01% accuracy), then $\delta y_2 / \delta y_1$ lies between 6 for the log function and 9 for the sin, cos and exp functions.

The above analysis shows that 6-9 times as many dividing lines must be used with (2.16) to get equivalent accuracy to (2.17a) for the first derivatives. Equation (2.16) requires about half as many computer multiplications, divisions, etc., compared to (2.17a) but this affects only one statement of the computer program and so is insignificant in terms of computer time. A similar saving in lines may be made by using the 5-point scheme (2.17b) instead of (2.5) for second derivatives. The superiority of the five line schemes over the three line schemes will be illustrated in Section 3.5.

2.7 Difference Formulas Applied Near a Boundary

To apply (2.17) on a line adjacent to a boundary line is not possible unless the boundary line is a line of symmetry when image lines are used. If the boundary line is not a line of symmetry then the following formulas are recommended.

(i) Dirichlet Boundary Condition

Use

$$\pm h \frac{\partial \psi_1}{\partial y} = \frac{1}{4}(\psi_1 - \psi_0) - \frac{3}{2}(\psi_1 - \psi_2) + \frac{1}{2}(\psi_1 - \psi_3)$$

$$- \frac{1}{12}(\psi_1 - \psi_4) + O(h^5 \psi^V) \qquad (2.19)$$

for a first derivative, where lines 0, 1, 2, 3, 4 are adjacent and line 0 forms the boundary. The symbols ψ_0, ψ_1, etc., refer to the values of ψ on line 0, line 1, etc., and ψ^V refers to the fifth derivative of ψ with respect to y in the range considered. The upper sign is used if the lines 0, 1, 2, 3, 4 are at increasing y values, otherwise the lower sign is used. For a second derivative

$$\frac{h^2}{2}\frac{\partial^2\psi_1}{\partial y^2} = -\frac{1}{6}(\psi_2-\psi_1) + \frac{1.75}{3}(\psi_3-\psi_1) - \frac{1}{4}(\psi_4-\psi_1)$$

$$+ \frac{0.125}{3}(\psi_5-\psi_1) + \frac{1.25}{3}(\psi_0-\psi_1) + O(h^6\psi^{VI}) \qquad (2.20)$$

is recommended.

(ii) Neumann and Mixed Boundary Conditions

In this case $\partial\psi/\partial y$ is a constant on the boundary or else $\partial\psi/\partial y$ is given as a function of ψ. In the latter case calculate $\partial\psi_0/\partial y$ from the boundary condition and then, for both cases, use

$$\pm h\frac{\partial\psi_1}{\partial y} = \frac{8.5}{9}(\psi_1-\psi_0) - \frac{1}{2}(\psi_1-\psi_2) + \frac{1}{18}(\psi_1-\psi_3) \mp \frac{1}{3}h\frac{\partial\psi_0}{\partial y} + O(h^5\psi^V) \qquad (2.21)$$

for a first derivative and

$$\frac{h^2}{2}\frac{\partial^2\psi_1}{\partial y^2} = \frac{3.5}{4}(\psi_2-\psi_1) - \frac{1}{9}(\psi_3-\psi_1) + \frac{0.0625}{6}(\psi_4-\psi_1)$$

$$+ \frac{8.03125}{9}(\psi_0-\psi_1) \pm \frac{0.625}{3}h\frac{\partial\psi_0}{\partial y} + O(h^6\psi^{VI}) \qquad (2.22)$$

for a second derivative. The appropriate ± sign is chosen in the same way as in (i) above.

Also the appropriate form for $\partial^2\psi_0/\partial y^2$ is given by

$$\frac{h^2}{2}\frac{\partial^2\psi_0}{\partial y^2} = 4(\psi_1-\psi_0 \mp h\frac{\partial\psi_0}{\partial y}) - 1.5\,(\psi_2-\psi_0 \mp 2h\frac{\partial\psi_0}{\partial y})$$

$$+ \frac{4}{9}(\psi_3-\psi_0 \mp 3h\frac{\partial\psi_0}{\partial y}) - \frac{1}{16}(\psi_4-\psi_0 \mp 4h\frac{\partial\psi_0}{\partial y})$$

$$+ O(h^6\psi^{VI}) \qquad (2.23)$$

In addition to first and second derivatives, formulas for higher derivatives may be found if required. For example, in the case of the Neumann boundary condition, $\partial^3\psi_1/\partial y^3$ can be determined by solving the equations

$$\psi_{n+1} - \psi_1 = nh\psi_1^I + \frac{(nh)^2}{2}\psi_1^{II} + \frac{(nh)^3}{3!}\psi_1^{III} + \frac{(nh)^4}{4!}\psi_1^{IV}$$

$$+ \frac{(nh)^5}{5!}\psi_1^V \qquad (n = -1,1,2,3),$$

$$h\frac{\partial\psi_0}{\partial y} = h\psi_1^I - h^2\psi_1^{II} + \frac{h^3}{2}\psi_1^{III} - \frac{h^4}{3!}\psi_1^{IV} + \frac{h^5}{4!}\psi_1^V$$

for ψ_1^{III} in terms of $\psi_0, \psi_1, \psi_2, \psi_3, \psi_4$ and $\partial\psi_0/\partial y$. Note that the required formula can be found conveniently by computer matrix inversion.

2.8 Other Geometries

For simplicity we used a rectangle to describe MOL. The application to the geometry of Figure 2.3 with polar co-ordinates is obvious; in this case lines ϕ = constant are used.

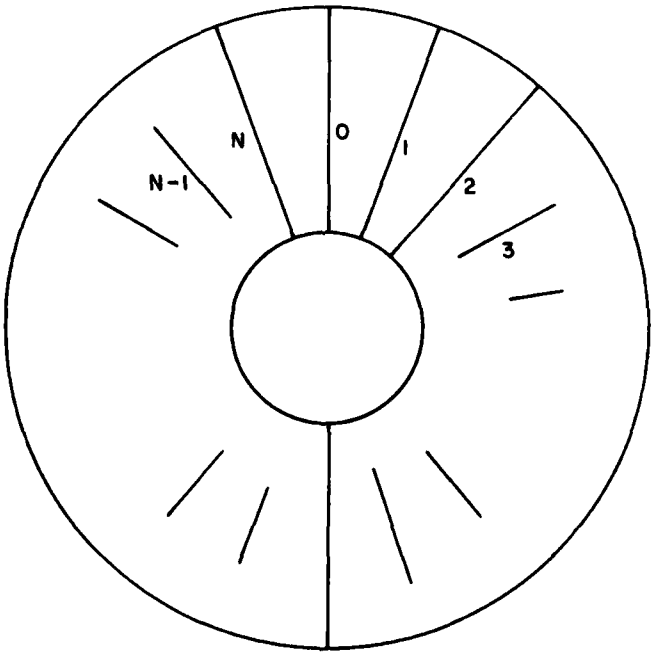

FIG. 2.3 MOL WITH POLAR CO-ORDINATES

Application of the method to more complicated geometries is generally limited only by the degree of ingenuity of the user, since an appropriate choice of co-ordinates and various transformations can be used to map most regions into one of the simple regions just mentioned. For example the region ABCD of Figure 2.4 can be mapped into the rectangle $0 \leqslant \xi \leqslant 1$, $0 \leqslant \eta \leqslant 1$ by the transformation

$$\xi = \frac{x - g_1(y)}{g_2(y) - g_1(y)}; \quad \eta = \frac{y - f_1(x)}{f_2(x) - f_1(x)}$$

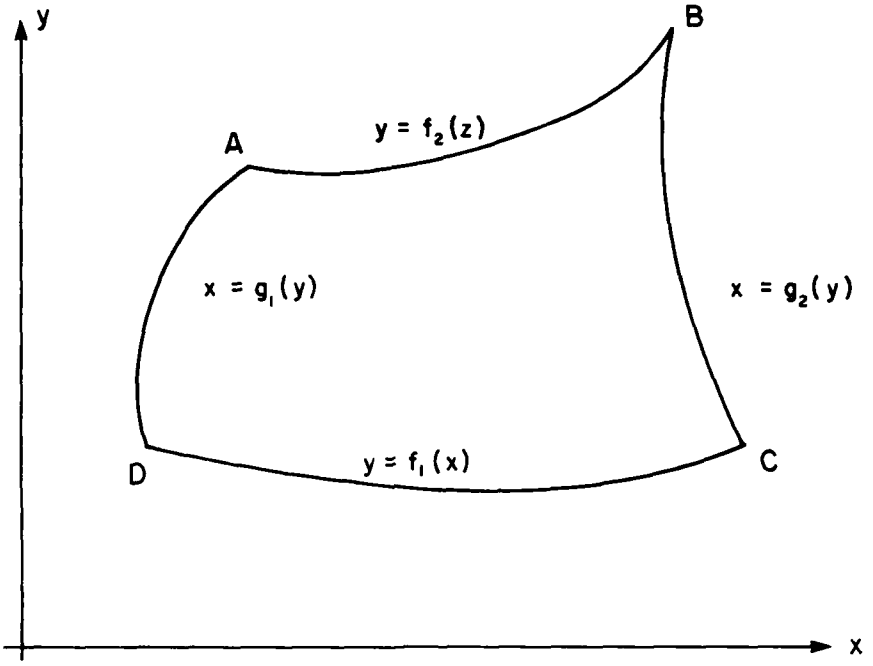

FIG. 2.4 THE REGION ABCD

This transformation is now applied to the partial differential equations using, for example,

$$\frac{\partial}{\partial x} = \xi_x \frac{\partial}{\partial \xi} + \eta_x \frac{\partial}{\partial \eta}$$

and

$$\frac{\partial^2}{\partial x^2} = \xi_{xx} \frac{\partial}{\partial \xi} + \eta_{xx} \frac{\partial}{\partial \eta} + \xi_x^2 \frac{\partial^2}{\partial \xi^2} + \eta_x^2 \frac{\partial^2}{\partial \eta^2} + 2\xi_x \eta_x \frac{\partial^2}{\partial \xi \partial \eta}$$

and then the resulting equations are solved by MOL in the (ξ,η) plane. Note that the transformation preserves linearity. Such a transformation is used to solve the conical flow problem of Section 4.3.

2.9 A Cautionary Note on the Instability

The preceding description of MOL is somewhat idealized in the sense that we have assumed that the computer round off errors, the discretisation error in the PMC integration scheme and also the instability inherent in the ordinary differential equations are negligible. They of course are not negligible; in fact it is known that MOL solutions are unstable since as more and more lines are used the solutions diverge and thus become meaningless. This fact may deter people from using MOL and one of our main purposes in this report is to show people that problems of physical interest have been solved successfully by MOL. We also present an analysis of the instability in the linear case in the next chapter. This analysis will show the form of the instability and thus the user will be made aware of what problems to expect. Then the same linear problem that is analysed is solved numerically by MOL. It will be seen that 4 or 5 significant figure accuracy is obtained.

Perhaps we should point out for the moment that MOL solutions may be compared to asymptotic series solutions since the latter are divergent series so that as more and more terms are taken the solutions become meaningless. However many useful results are obtained with asymptotic series using only a few terms.

Also parallel shooting methods (Keller 1968) may be used to overcome the instability. In these methods we subdivide the total range of integration $0 \leqslant x \leqslant a$ into subintervals and 'shoot', for example, as shown diagrammatically in Figure 2.5 below. Of course the number of unknowns is increased in this case since we have to estimate values at $x = 0$, $x = a/2$ and $x = a$. In the linear case the total computational time will be practically the same as using the one complete range since the number of unknowns is increased by a factor of four but each integration to get the derivatives $\frac{\partial \epsilon_i}{\partial F_j}$ is over the range a/4. Of course the time involved in solving the linear system (2.10) or (2.13) would eventually become large if many subintervals were used.

The parallel shooting method is used on our linear example in Section 3.5.2.

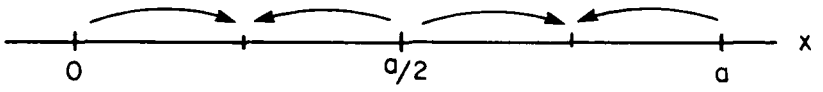

FIG. 2.5 PARALLEL SHOOTING RANGES

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CHAPTER 3.0 STABILITY AND CONVERGENCE OF MOL

3.1 Introduction

In the first part of this chapter Hadamard's example of the Cauchy problem for the Laplace equation in a rectangle is discussed. This example shows that we may expect MOL to be inherently unstable.

A closer analysis of MOL, using the scheme (2.4), for the Laplace equation in a rectangle is then made. This analysis shows that the general solution by MOL is comprised of two parts. The first of these is an unwanted solution which is negligible for sufficiently small x (the continuous variable) or when sufficiently few lines are used but which otherwise grows large. The second part of the general MOL solution is the required solution which tends to the exact solution as the y increment tends to zero (i.e. as the number of lines increases).

In the final part the stability and convergence of MOL is illustrated with a linear example. It will be seen that good accuracy (4 significant figures) is obtained with a suitable choice of both number of lines and integration step size δx.

3.2 Hadamard's Example

Hadamard (1952) investigates the solution of Laplace's equation and shows that, subject to Cauchy data of a certain type, the solution is not well behaved since it will oscillate between very large positive and negative values when the correct solution, in the limit of vanishing Cauchy data, should be zero. Hadamard poses the example

$$\psi_{xx} + \psi_{yy} = 0 \tag{3.1}$$

with Cauchy data given at the line $x = 0$,

$$\psi(0,y) = 0,$$

$$\psi_x(0,y) = A_n \sin ny, \tag{3.2}$$

where n is large and A_n is a function of n which grows small as n grows large (e.g., n^{-p}, $p > 0$). The solution to this problem is

$$\psi(x,y) = (A_n/n) \sin ny \sinh nx \tag{3.3}$$

The sinh nx factor is large because of the growth of e^{nx}. The sin ny factor causes oscillation of the function with varying y. Hence however close to zero we choose to make the Cauchy data (i.e., n large) the solution $\psi(x,y)$ will not be zero but will oscillate between large positive and negative values. Since zero is the solution of (3.1) with vanishing Cauchy data ($A_n = 0$) we conclude that for Laplace's equation the dependence of the solution on the initial data is not in general continuous.

Garabedian (1964) concludes also that the above problem is not correctly set or well posed. He defines a boundary-value problem for a partial differential equation, or for a system of partial differential equations, to be correctly set in the sense of Hadamard if and only if its solution exists, is unique, and depends continuously on the data assigned.

Consider now Hadamard's example in the context of MOL. We may proceed with MOL by estimating $\psi_x(0,y)$ and using this estimate integrate (3.1) numerically away from x = 0. After iteration we arrive at a numerical solution of $\psi_x(0,y)$. Suppose the exact solution to the problem is zero, i.e., $\psi_x(0,y) = 0$, but that due to discretization and round-off errors the value of $\psi_x(0,y)$ is of order 10^{-10}. Then the situation is similar to n being large in (3.2) in the sense that A_n is not quite zero. As we integrate numerically in MOL away from x = 0 the solution will be in a form similar to (3.3) and will thus become large and oscillatory for sufficiently large x. Thus we cannot obtain a good approximation to the exact solution unless x is small.

It may also be noted that in the general case when solving by MOL even an exact $\psi_x(0,y)$ cannot give a good solution for all x. The reason for this is that the x discretization error introduces an unwanted solution equivalent to $A_n \neq 0$ in the Hadamard example. Thus the instability is always present but its contribution may be insignificant for x sufficiently small.

The above observations of instability are analyzed more closely in the next part of this chapter. It will be confirmed that a reasonably accurate solution may be obtained if x is sufficiently small. It will also be shown that the instability is worse if too many lines are used.

3.3 Analysis of Stability of MOL

To illustrate the stability and convergence consider the problem of solving Laplace's equation

$$\psi_{xx} + \psi_{yy} = 0 \tag{3.4}$$

in a rectangular domain $0 \leqslant x \leqslant 1$, $-b \leqslant y \leqslant b$, with the following Dirichlet boundary conditions:

$$\psi(0,y) = \psi(1,y) = 0, \tag{3.5}$$

$$\psi(x,b) = \psi(x,-b) = \sin \pi x \tag{3.6}$$

The exact solution for this problem is known to be

$$\psi(x,y) = \frac{\cosh \pi y \sin \pi x}{\cosh \pi b} \tag{3.7}$$

We now consider the solution of this problem by MOL. Since the problem contains the two lines of symmetry x = ½ and y = 0, we can reduce the region of interest to the upper left quadrant of the rectangle, i.e. $0 \leqslant x \leqslant ½$, $0 \leqslant y \leqslant b$. N - 1 interior lines are drawn parallel to the x axis with equal spacing h = b/N, so that

$$y_n = nh = nb/N \tag{3.8}$$

The symmetry conditions

$$\psi_x(\tfrac{1}{2},y) = 0, \tag{3.9}$$

$$\psi(x,-y) = \psi(x,y), \tag{3.10}$$

are applied.

To get some insight into the stability and convergence of MOL the three-point formula (2.5) is used to approximate ψ_{yy} in (3.4) giving

$$\psi_n'' + (\psi_{n+1} - 2\psi_n + \psi_{n-1})/h^2 = 0 \qquad (n = 0,1,2,\ldots,N-1) \tag{3.11}$$

where $\psi_n(x)$ is the approximation for $\psi(x,y_n)$ and the primes indicate differentiation with respect to x. To the system (3.11) we add the appropriate boundary and symmetry conditions,

$$\psi_n(0) = 0, \tag{3.12}$$

$$\psi_n'(\tfrac{1}{2}) = 0, \tag{3.13}$$

$$\psi_N = \sin \pi x, \tag{3.14}$$

$$\psi_{-n}(x) = \psi_n(x), \qquad n = 1,2,\ldots,N-1 \tag{3.15}$$

3.3.1 Complementary Function

To obtain the complete solution of (3.11)-(3.15) we first look for the complementary function. This function must satisfy (3.11), (3.15) and also

$$\psi_N = 0 \tag{3.16}$$

We attempt a solution

$$\psi_n(x) = C_n e^{\mu x}$$

and substitute into (3.11) to give the recurrence relation

$$C_{n+1} - 2z\,C_n + C_{n-1} = 0 \tag{3.17}$$

where

$$z = 1 - \frac{\mu^2 h^2}{2}$$

For the complementary function to satisfy (3.15) requires $C_{-1} = C_1$ and thus using (3.17) we obtain, for C_0 arbitrary,

$$\begin{aligned} C_1 &= z \cdot C_0 = T_1(z)C_0 \\ C_2 &= 2zC_1 - C_0 = (2z^2 - 1)C_0 = T_2(z)C_0 \\ C_3 &= 2zC_2 - C_1 = 2z(2z^2 - 1)C_0 - zC_0 = (4z^3 - 3z)C_0 = T_3(z)C_0 \\ &\cdots \\ C_N &= T_N(z)C_0 \end{aligned} \tag{3.18}$$

where $T_n(z)$ is the Chebyshev polynomial of order n. Now to satisfy (3.16), since $C_0 \neq 0$, we have

$$0 = T_N(z) = \cos N\theta$$

where $z = \cos\theta$. Thus θ takes on discrete values given by θ_m where

$$N\theta_m = \frac{m\pi}{2} \text{ for } m = 1,3,\ldots,2N-1$$

Also

$$1 - \frac{\mu_m^2 h^2}{2} = z_m = \cos\theta_m = 1 - 2\sin^2\frac{\theta_m}{2} = 1 - 2\sin^2\frac{m\pi}{4N}$$

and so

$$|\mu_m| = \frac{2}{h}\sin\frac{m\pi}{4N} \tag{3.19}$$

Taking a linear combination of the allowable solution and using the fact that $T_n(z) = \cos n\theta$ gives us the complete complementary function

$$\psi_n^{(c)}(x) = \sum_{m=1,3\ldots}^{2N-1} \cos\frac{nm\pi}{2N}\left(A_m e^{\mu_m x} + B_m e^{-\mu_m x}\right) \tag{3.20}$$

for constants A_m, B_m.

3.3.2 Particular Integral

In this case we follow a similar procedure to that of finding the complementary function except that we attempt a solution

$$\psi_n(x) = C_n \sin \pi x \tag{3.21}$$

and obtain the recurrence relation

$$C_{n+1} - 2z\,C_n + C_{n-1} = 0$$

where $z = 1 + \pi^2 h^2/2$. Thus we obtain the same relations (3.18), and since we now require $\psi_N = \sin \pi x$ we have

$$C_N = T_N(z)C_0 = 1$$

or

$$C_0 = \frac{1}{T_N(z)}$$

On putting $\cosh \theta = z$ and using the fact that $T_n(\cosh \theta) \equiv \cosh n\theta$, the particular integral (3.21) becomes

$$\psi_n^{(p)}(x) = \frac{\cosh n\theta}{\cosh N\theta} \sin \pi x \tag{3.22}$$

where $\cosh \theta = 1 + \pi^2 h^2/2$.

The complete solution to our problem is then

$$\psi_n(x) = \psi_n^{(p)}(x) + \psi_n^{(c)}(x)$$

3.3.3 Instability in the Method of Lines

Clearly the solution we require by MOL is the particular integral (3.22). The complementary function (3.20), in order to satisfy the boundary conditions (3.12) and (3.13), requires $A_m = B_m = 0$ for all m. However in solving the problem numerically it may be that, due to computer round off and discretization errors in the numerical integration, the A_m and B_m are not quite zero. In this case we may expect a large growth of the unwanted solution $A_m e^{\mu_m x}$ in (3.20) since $\mu_m x$ may grow rather large. The size of the unwanted term and its form can be investigated by looking at the largest contribution in (3.20). This is found by setting $m = 2N - 1$ since then

$$\mu_m = \frac{2}{h}\sin\left(\frac{\pi}{2} - \frac{\pi}{4N}\right) = \frac{2}{h}\cos\frac{\pi}{4N} = \frac{2N}{b}\cos\frac{\pi}{4N}$$

Thus, since N is normally greater than 3, $\mu_m \simeq 2N/b$ and the unwanted growth in $\psi_n^{(c)}(x)$ is

$$G_{2N-1} \simeq A_{2N-1} \cos n\pi \left(1 - \frac{1}{2N}\right) e^{2Nx/b}$$

The cosine factor is approximately unity in magnitude thus

$$|G_{2N-1}| \simeq A_{2N-1} \exp\left(\frac{2Nx}{b}\right) \tag{3.23}$$

It can be seen that the gradient $d/dx[\psi_n^{(c)}(x)]$ will grow even more rapidly since this will be given by

$$|G'_{2N-1}| \simeq A_{2N-1} \frac{2N}{b} \exp\left(\frac{2Nx}{b}\right) \tag{3.24}$$

In our particular problem we really require $\psi'_n(\frac{1}{2}) = 0$ to give symmetry about $x = \frac{1}{2}$ but it can be seen from (3.24) that if A_{2N-1} is not quite zero and if the product Nx is sufficiently large then it would be impossible to satisfy the symmetry condition.

Now due to the truncation errors of a finite word length machine the initial conditions at $x = 0$ are not, in general, stored exactly. This would have the effect of A_m and B_m being not quite zero and so lead to the instability.

Also, even with an infinite word length machine, the discretization errors of the numerical integration scheme will cause instability. This can be seen by considering the first step from $x = 0$ to $x = \delta x$ using the exact conditions at $x = 0$ i.e. $\psi_n(0) = 0$ and $\psi'_n(0) = \pi \cosh n\theta/\cosh N\theta$. We obtain a numerical solution at $x = \delta x$ given by

$$\psi_n = \psi_n(\text{exact}) + \epsilon_n$$

$$\psi'_n = \psi'_n(\text{exact}) + \delta_n$$

where ϵ_n, δ_n are the errors due to numerical integration. Thus the A_m and B_m now satisfy

$$\sum_m \cos\frac{nm\pi}{2N}\left(A_m e^{\mu_m \delta x} + B_m e^{-\mu_m \delta x}\right) = \epsilon_n$$

$$\sum_m \mu_m \cos\frac{nm\pi}{2N}\left(A_m e^{\mu_m \delta x} - B_m e^{-\mu_m \delta x}\right) = \delta_n$$

so clearly A_m and B_m are not zero and we again have an instability problem.

We have thus shown that instability is unavoidable but we do not know how serious it is until we attempt solutions to practical problems. Since we now know the form of the unstable term (3.23) or (3.24) we can at least hope to minimize its effect.

For instance, since it is the product Nx which causes instability, it may in some cases be worthwhile using smaller integration distances x. This leads to the idea of the parallel shooting technique mentioned at the end of Chapter 2. Also using a higher (than second) order difference scheme for the ψ_{yy} derivative enables us to use fewer lines (N) to achieve the same accuracy for this second derivative. In turn by using N smaller we reduce the exponential growth in (3.23) or (3.24). For example the fourth order accurate scheme using five adjacent lines could be used. This scheme was considered in Section 2.6 and its numerical application is covered in Section 3.5.3.

Notice that although the instability is unavoidable it is no worse than other similar techniques, used particularly in the Soviet Union, such as Telenin's method (see Gilinskii et al. (1964)) or the Method of Integral Relations (MIR). Indeed it can be shown that the instability of MIR is likely to be much worse than that of MOL. In Appendix A the MIR instability term similar to (3.24) is derived and shown to be

$$A_{2N-1} \exp\left(\frac{4N^2}{\pi b}\right) \tag{3.25}$$

at x = ½. The functions (3.24) and (3.25), without the A_{2N-1}, are tabulated in Table I for x = ½ and b = 0.475 (the value used in our example later). From this table it can be seen that instability of MIR is significantly worse.

Even so MIR has been used successfully in the Soviet Union and also by Holt (1977) for many years. In Chapter 5 of Holt's book application of MIR to several problems such as the supersonic blunt body problem and the laminar boundary layer equations is explained.

3.4 Convergence of the Particular Integral

It is of interest to compare the particular integral (3.22) with the exact solution (3.7). This is accomplished by expanding the inverse hyperbolic function in $\theta = \cosh^{-1}(1 + \pi^2 h^2/2)$ giving

$$\theta = \pi h \left[1 - \frac{\pi^2 h^2}{24} + 0(h^4)\right]$$

and then expanding the particular integral in a Taylor series about h = 0

$$\psi_n(x) = \frac{\cosh \pi y_n}{\cosh \pi b} \sin \pi x \left[1 + \frac{\pi^3 b^3}{24N^2}\left(\tanh \pi b - \frac{y_n}{b} \tanh \pi y_n\right) + 0(N^{-4})\right]$$

Thus the particular integral converges to the exact solution (3.7) and has error $0(N^{-2})$. This error is expected since we use a formula of $0(h^2)$ accuracy for the second derivative ψ_{yy} and $h = \frac{b}{N}$.

3.5 A Linear Example to Illustrate the Stability and Convergence

In this section we solve numerically the problem posed in Section 3.3 and given by Equations (3.4)-(3.6) using b = 0.475. The exact solution (3.7) is tabulated in Table II for values of x = 0.125, 0.25, 0.375, 0.5 and for values of y = 0, 0.475/3 and 2/3 × 0.475; also shown are values of $\psi_x(x = 0)$ at the above y values.

We will use the three line difference scheme (2.5) in order to get a better understanding of the stability since in this case we know the analytic MOL solution is given by (3.22). With the three line scheme we will investigate the effects of parallel shooting, of varying the number of lines, and of varying the integration step size δx.

We will then use the five line scheme and show that accurate solutions can be obtained using only a few lines.

3.5.1 The Three Line Analytical Solution

Let us consider the analytical solution to the MOL equations which is given by the particular integral (3.22) of the ordinary differential Equations (3.11). This analytical solution represents the best we can hope to achieve numerically since it does not contain any round off or discretization errors and hence the complementary function (3.20) is zero. Remember that, numerically, we expect (3.20) to be non zero and hence to cause some inaccuracy. The extent of the inaccuracy is what we want to observe. Thus comparison of our numerical solution with the analytical MOL solution, rather than with the exact solution (3.7), is more meaningful at this stage. The analytical MOL solution is given in Table III at the same x and y values as listed for Table II; we present results for N = 3,6,9,12 and 15 (i.e. the number of lines used to divide the region $0 \leqslant y \leqslant b$ into strips).

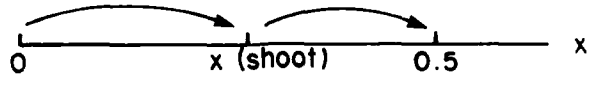
3.5.2 The Three Line Numerical Scheme

This section is split into three parts which illustrate three different ways of overcoming the instability.

The present results are obtained using the Runge Kutta Gill integration method which has truncation error $0(\delta x^5)$. One step of the Newton iteration scheme (2.10) is used to find the missing initial conditions. In the tables to follow we print values of ψ and the initial slopes $\psi_x(x = 0)$ at the (x,y) values mentioned in Section (3.5). We also print N (the number of lines), the integration step size DELX, and the matching point XSHOOT used in the parallel shooting technique. If XSHOOT = 0.5 then only one shooting range is used and we print out the SUM SQUARES GRADIENTS which represents Σp_i^2 at x = 0.5 where $p_i \equiv \partial\psi_i/\partial x$; because of symmetry about x = 0.5 this quantity should be zero. If XSHOOT ≠ 0.5 then two shooting ranges have been used as shown below.

(a) **Effect of Varying the Length of Shooting** (Parallel Shooting)

In order to help to overcome the instability we can use a parallel shooting technique as shown diagrammatically below.



We first estimate $p_i(0)$, integrate the differential equations from 0 to x(shoot) and obtain values ψ_i^S and p_i^S, say, on line i at x = x(shoot). Also using estimates of ψ_i and p_i at x = x(shoot) (designated ψ_i^{SH} and p_i^{SH} say) we integrate the ordinary differential equations to the end of the range x = 0.5 where we obtain values of $p_i = p_i(0.5)$.

Be suitably choosing $p_i(0)$, ψ_i^{SH} and p_i^{SH} we hope to solve the system of equations

$$\left.\begin{aligned} p_i(0.5) &= 0 \qquad \text{(symmetry about } x = 0.5) \\ \left.\begin{aligned} \psi_i^S - \psi_i^{SH} &= 0 \\ p_i^S - p_i^{SH} &= 0 \end{aligned}\right\} &\quad \text{matching at } x = x(\text{shoot}) \end{aligned}\right\} \tag{3.26}$$

The optimum choice of $p_i(0)$, ψ_i^{SH} and p_i^{SH} is made using Newton's method (2.10). Our linear illustrative problem remains linear since the matching conditions at x = x(shoot) are linear. Thus one step in the above method is all that is required.

Table IV shows the results of varying x(shoot) with N = 15 and $\delta x = 1/32$. It can be seen that instability is least when using the smallest shooting range (i.e. x(shoot) = 0.25). Shooting the whole range is clearly hopeless while using x(shoot) = 0.125 or 0.375 gives fairly reasonable results. Using x(shoot) = 0.25 gives good stability and hence a solution accurate to almost 4 figures compared to the analytic MOL solution given in Table III. The quantity SUM SQUARES RESIDUALS printed in the tables represents the sum of squares of the left hand sides of (3.26). The two entries given for x = x(shoot) list values of ψ_i^S (obtained after integration from zero) and ψ_i^{SH} (the best values of ψ_i(XSHOOT) to minimize the RESIDUALS of (3.26)).

(b) Effect of Varying the Integration Step Length δx

It has been shown that the instability is caused by terms of the type $\exp(\mu_{2N-1}\, x)$. On integrating numerically by the Runge Kutta Gill method we find that after k steps the term $\exp(\mu_{2N-1}\, k\, \delta x)$ is represented by E^k where

$$E = 1 + \Delta + \frac{\Delta^2}{2!} + \frac{\Delta^3}{3!} + \frac{\Delta^4}{4!}$$

and $\Delta = \mu_{2N-1}\, \delta x$. Thus the error grows in the numerical integration like E^k rather than $\exp(k\Delta)$. E^k is always less than $\exp(k\Delta)$ for $\Delta > 0$ and the ratio $E^k/\exp(k\Delta)$ shrinks rapidly with increasing Δ. For example when $\delta x = 1/4$ (i.e. k = 2 for integration over the whole range) $E^k/\exp(k\Delta)$ is about 10^{-4} for N = 12.

Thus we may expect instability to improve as Δx is increased (but of course the particular integral would not be so accurately represented).

Table V shows the improvement in stability for N = 15 and x(shoot) = 0.5. We can see that we progress from the unstable cases of $\delta x = 1/32$ or 1/16 to a fairly stable solution with $\delta x = 1/8$ and to a stable solution with $\delta x = 1/4$. Referring to accuracy the latter two solutions are reasonably good except at the point x = 1/2, y = 2/3* 0.475.

(c) Effect of Varying the Number of Lines

It can be seen from Table VI that the effect of decreasing the number of lines improves enormously the behaviour of the instability. The N = 15 solution is hopelessly unstable, while using N = 12 gives a mildly unstable situation (the results are not accurate compared to the analytical MOL solution of Table III). Using N = 9, 6 or 3 stability does not seem to

be any problem and the accuracy of the solution is very good compared to the analytic MOL solution (although not necessarily compared to the exact solution given in Table II).

To get good accuracy compared to the exact solution using the 3 line difference scheme we would clearly have to use many lines (N = 57 would give 4 decimal figures accuracy) but this, numerically, would give instability. Thus we clearly must use a higher order difference scheme to represent the derivatives so that we can minimize the number of lines necessary to achieve an accurate representation of the particular integral. This scheme is now investigated numerically.

3.5.3 The Five Line Numerical Scheme

As we saw from the three line scheme applied to our linear example we can expect good stability with $N \leqslant 9$ but the accuracy may not be sufficiently accurate. To keep the stability and also get accuracy we consider the fourth order accurate scheme using (2.17b) to represent the derivative ψ_{yy} (with (2.20) used next to the boundary line y = b). This time we only consider shooting the one range $0 \leqslant x \leqslant 0.5$ since sufficient accuracy and stability is obtained in this case (using $N \leqslant 9$).

Table VII lists values of ψ and the initial slopes $\psi_x(x = 0)$ for some values of N and δx. It can be seen, by comparing with Table II, that almost 4 significant figure accuracy is obtained using N = 6 and $\delta x = 0.0625$. Notice also that using the coarsest scheme, N = 3 and $\delta x = 0.25$, produces results with at worst 2% error in ψ and 1% error in the initial slopes. The N = 12 results again indicate instability when δx is too small.

In terms of computer time the method is very efficient as can be seen from the N = 6, $\delta x = 0.0625$ solution. This required only 0.3 seconds on an IBM 3032 computer. The efficiency is confirmed by further computer times quoted in the nonlinear examples covered in the next chapter.

3.6 Summary

The three line scheme (2.5) to represent the derivative has been used mainly to illustrate the instability inherent in the method of lines. It has been confirmed that three techniques help to overcome the instability but the latter two decrease the accuracy of the particular integral which we seek to obtain. It has been shown that, for our linear example, the higher order difference scheme using five adjacent lines (2.17) gives an accurate representation of the particular integral while at the same time giving a stable solution. Thus use of the five line scheme is always recommended.

Notice also that three line schemes of order (N^{-4}) accuracy in the particular integral may be used in certain cases. These schemes are given in Appendix B; they require calculating the derivatives p_i in the ordinary differential equations by solution of a tridiagonal system of equations. This can be achieved efficiently by the Thomas algorithm (von Rosenburg, 1969).

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TABLE I

TABLE OF THE FUNCTIONS (3.24) AND (3.25) USING b = 0.475 TO ILLUSTRATE THE INSTABILITY OF MOL AND OF THE METHOD OF INTEGRAL RELATIONS FOR N TOO LARGE

N	(3.24)	(3.25)
2	5.7, 2	4.5, 4 ($\equiv 4.5 \times 10^4$)
3	7.0, 3	3.0, 10
4	7.6, 4	4.2, 18
5	7.8, 5	1.3, 29
6	7.7, 6	8.1, 41
9	6.4, 9	$>10^{75}$
12	4.7, 12	$>10^{75}$

TABLE II

EXACT SOLUTION TO MOL LINEAR PROBLEM

X	Y = 0	0.475/3	2*0.475/3
0.125	0.1638	0.1845	0.2518
0.250	0.3027	0.3409	0.4653
0.375	0.3955	0.4454	0.6079
0.500	0.4281	0.4821	0.6580
INITIAL SLOPES	1.3449	1.5147	2.0671

TABLE III

ANALYTICAL MOL SOLUTIONS GIVEN BY 3.22

N = 3

X	Y = 0	0.475/3	2*0.475/3
0.125	0.1660	0.1866	0.2533
0.250	0.3068	0.3448	0.4680
0.375	0.4009	0.4505	0.6115
0.500	0.4339	0.4876	0.6619
INITIAL SLOPES	1.3632	1.5318	2.0794

N = 6

X	Y = 0	0.475/3	2*0.475/3
0.125	0.1644	0.1850	0.2522
0.250	0.3037	0.3419	0.4660
0.375	0.3969	0.4467	0.6088
0.500	0.4296	0.4835	0.6590
INITIAL SLOPES	1.3495	1.5190	2.0702

N = 9

X	Y = 0	0.475/3	2*0.475/3
0.125	0.1641	0.1847	0.2520
0.250	0.3032	0.3414	0.4656
0.375	0.3961	0.4460	0.6083
0.500	0.4287	0.4828	0.6584
INITIAL SLOPES	1.3469	1.5166	2.0685

N = 12

X	Y = 0	0.475/3	2*0.475/3
0.125	0.1640	0.1846	0.2519
0.250	0.3030	0.3412	0.4654
0.375	0.3958	0.4458	0.6081
0.500	0.4285	0.4825	0.6582
INITIAL SLOPES	1.3460	1.5158	2.0679

N = 15

X	Y = 0	0.475/3	2*0.475/3
0.125	0.1639	0.1846	0.2519
0.250	0.3029	0.3411	0.4654
0.375	0.3957	0.4456	0.6080
0.500	0.4283	0.4824	0.6581
INITIAL SLOPES	1.3456	1.5154	2.0676

TABLE IV

EFFECT OF VARYING X(SHOOT)

N = 15 DELX = 0.03125 XSHOOT = 0.125

X	Y = 0	0.475/3	2*0.475/3
0.125	0.1635	0.1840	0.2511
0.125	0.1635	0.1840	0.2511
0.250	0.3023	0.3401	0.4630
0.375	0.3955	0.4452	0.6015
0.500	0.4284	0.4833	0.6315
INITIAL SLOPES	1.3422	1.5108	2.0623

SUM SQUARES RESIDUALS 6.885D 02

N = 25 DELX = 0.03125 XSHOOT = 0.250

X	Y = 0	0.475/3	2*0.475/3
0.125	0.1639	0.1846	0.2519
0.250	0.3029	0.3411	0.4654
0.250	0.3029	0.3411	0.4654
0.375	0.3958	0.4457	0.6081
0.500	0.4284	0.4824	0.6582
INITIAL SLOPES	1.3457	1.5155	2.0677

SUM SQUARES RESIDUALS 1.609D-04

N = 25 DELX = 0.03125 XSHOOT = 0.375

X	Y = 0	0.475/3	2*0.475/3
0.125	0.1657	0.1860	0.2526
0.250	0.3072	0.3441	0.4667
0.375	0.4028	0.4701	0.6643
0.375	0.4075	0.4500	0.6099
0.500	0.4354	0.4870	0.6601
INITIAL SLOPES	1.3595	1.5265	2.0732

SUM SQUARES RESIDUALS 6.799D 01

N = 15 DELX = 0.03125 XSHOOT = 0.500

X	Y = 0	0.475/3	2*0.475/3
0.125	0.0363	0.0805	0.1980
0.250	0.0129	0.1170	0.3574
0.375	-0.1656	0.0768	0.4544
0.500	0.6212	-8.3976	-1.2045
INITIAL SLOPES	0.3648	0.7049	1.6394

SUM SQUARES GRADIENTS 1.050D 06

TABLE V

EFFECT OF VARYING δx

N = 15 DELX = 0.06250 XSHOOT = 0.500

X	Y = 0	0.475/3	2*0.475/3
0.125	0.1583	0.1812	0.2510
0.250	0.2873	0.3347	0.4649
0.375	0.3473	0.4450	0.6011
0.500	0.5551	1.0065	0.0971
INITIAL SLOPES	1.3044	1.4881	2.0591

SUM SQUARES GRADIENTS 3.905D 03

N = 15 DELX = 0.12500 XSHOOT = 0.500

X	Y = 0	0.475/3	2*0.475/3
0.125	0.1636	0.1843	0.2516
0.250	0.3022	0.3406	0.4652
0.375	0.3944	0.4448	0.6249
0.500	0.4260	0.4838	7.1353
INITIAL SLOPES	1.3435	1.5136	2.0653

SUM SQUARES GRADIENTS 8.146D-02

N = 15 DELX = 0.25000 XSHOOT = 0.500

X	Y = 0	0.475/3	2*0.475/3
0.250	0.3035	0.3413	0.4638
0.500	0.4302	0.4874	0.7246
INITIAL SLOPES	1.3500	1.5165	2.0533

SUM SQUARES GRADIENTS 7.961D-07

TABLE VI

EFFECT OF VARYING THE NUMBER OF LINES

N = 15 DELX = 0.03125 XSHOOT = 0.500

X	Y = 0	0.475/3	2*0.475/3
0.125	0.0363	0.0805	0.1980
0.250	0.0129	0.1170	0.3574
0.375	-0.1656	0.0768	0.4544
0.500	0.6212	-8.3976	-1.2045
INITIAL SLOPES	0.3648	0.7049	1.6394

SUM SQUARES GRADIENTS 1.050D 06

N = 12 DELX = 0.03125 XSHOOT = 0.500

X	Y = 0	0.475/3	2*0.475/3
0.125	0.1612	0.1824	0.2507
0.250	0.2967	0.3363	0.4631
0.375	0.3836	0.4381	0.6047
0.500	0.3944	0.5251	0.6659
INITIAL SLOPES	1.3249	1.4983	2.0586

SUM SQUARES GRADIENTS 2.130D 01

N = 9 DELX = 0.03125 XSHOOT = 0.500

X	Y = 0	0.475/3	2*0.475/3
0.125	0.1641	0.1848	0.2520
0.250	0.3032	0.3414	0.4656
0.375	0.3962	0.4460	0.6083
0.500	0.4289	0.4826	0.6585
INITIAL SLOPES	1.3470	1.5167	2.0685

SUM SQUARES GRADIENTS 2.326D-04

N = 6 DELX = 0.03125 XSHOOT = 0.500

X	Y = 0	0.475/3	2*0.475/3
0.125	0.1644	0.1850	0.2522
0.250	0.3037	0.3419	0.4660
0.375	0.3969	0.4467	0.6088
0.500	0.4296	0.4835	0.6590
INITIAL SLOPES	1.3495	1.5190	2.0702

SUM SQUARES GRADIENTS 3.526D-09

N = 3 DELX = 0.03125 XSHOOT = 0.500

X	Y = 0	0.475/3	2*0.475/3
0.125	0.1660	0.1866	0.2533
0.250	0.3068	0.3448	0.4680
0.375	0.4009	0.4505	0.6115
0.500	0.4339	0.4876	0.6619
INITIAL SLOPES	1.3632	1.5318	2.0794

SUM SQUARES GRADIENTS 1.841D-16

TABLE VII

NUMERICAL SOLUTION OF LINEAR PROBLEM BY THE FIVE LINE SCHEME

N = 3 DELX = 0.25000 XSHOOT = 0.500

X	Y = 0	0.475/3	2*0.475/3
0.250	0.3034	0.3412	0.4648
0.500	0.4306	0.4921	0.6469
INITIAL SLOPES	1.3497	1.5164	2.0532

SUM SQUARES GRADIENTS 1.579D-15

N = 6 DELX = 0.25000 XSHOOT = 0.500

X	Y = 0	0.475/3	2*0.475/3
0.250	0.3033	0.3412	0.4637
0.500	0.4298	0.4861	0.6695
INITIAL SLOPES	1.3492	1.5158	2.0528

SUM SQUARES GRADIENTS 1.845D-12

N = 6 DELX = 0.12500 XSHOOT = 0.500

X	Y = 0	0.475/3	2*0.475/3
0.125	0.1639	0.1845	0.2517
0.250	0.3028	0.3410	0.4658
0.375	0.3956	0.4458	0.6101
0.500	0.4286	0.4851	0.6671
INITIAL SLOPES	1.3453	1.5150	2.0660

SUM SQUARES GRADIENTS 7.634D-10

N = 6 DELX = 0.06250 XSHOOT = 0.500

X	Y = 0	0.475/3	2*0.475/3
0.125	0.1638	0.1845	0.2518
0.250	0.3027	0.3409	0.4653
0.375	0.3955	0.4455	0.6079
0.500	0.4281	0.4822	0.6581
INITIAL SLOPES	1.3449	1.5147	2.0671

SUM SQUARES GRADIENTS 6.791D-09

N = 12 DELX = 0.25000 XSHOOT = 0.500

X	Y = 0	0.475/3	2*0.475/3
0.250	0.3033	0.3412	0.4636
0.500	0.4299	0.4869	0.7121
INITIAL SLOPES	1.3493	1.5158	2.0528

SUM SQUARES GRADIENTS 6.444D-08

N = 12 DELX = 0.12500 XSHOOT = 0.500

X	Y = 0	0.475/3	2*0.475/3
0.125	0.1643	0.1849	0.2519
0.250	0.3038	0.3418	0.4657
0.375	0.3975	0.4470	0.5882
0.500	0.4329	0.4478	1.3762
INITIAL SLOPES	1.3488	1.5179	2.0675

SUM SQUARES GRADIENTS 2.295D-02

N = 12 DELX = 0.06250 XSHOOT = 0.500

X	Y = 0	0.475/3	2*0.475/3
0.125	0.1517	0.1746	0.2466
0.250	0.2753	0.3196	0.4550
0.375	0.3426	0.4112	0.5951
0.500	0.4644	0.5786	0.7017
INITIAL SLOPES	1.2519	1.4376	2.0260

SUM SQUARES GRADIENTS 3.962D 02

CHAPTER 4.0 TWO NONLINEAR EXAMPLES

4.1 Introduction

The linear problem covered in the last chapter was relatively easy to solve since only one step in the Newton scheme was required to obtain a solution. In nonlinear cases we have to be much more careful about initial estimates and we must be sure of using an efficient numerical optimisation scheme in order to find the optimum unknown values. It is believed that the method due to Powell (1965) is one of the most efficient methods (see Section 2.3 for a further coverage of Powell's method) for minimizing a sum of squares of nonlinear functions and as such is used in most of our computations presented here, the exception being the delta wing computations of Klunker et al. (1971) who used the modified Newton scheme mentioned in Section 2.2.2.

The first example is a structural problem and as such has been solved by the finite element method (Dixon 1971); MOL results are compared with the finite element solution.

The second example is a conical flow problem encountered in aerodynamics. We solve the full Euler equations comprising five simultaneous partial differential equations and also determine the location of the shock wave attached to the cone apex (see Fig. 4.3). A finite difference solution of the elliptic equations would be very time consuming and the earlier methods of solving this problem considered the complete hyperbolic system using the cone axis as the time-like direction. Comparisons of the MOL solution to the hyperbolic marching method (Babenko 1966; Gonidou 1968) are made. It is found that MOL solutions are some fifty times quicker while obtaining results of equal accuracy. The MOL results for a circular cone have been tabulated in AGARDograph 137 (Jones 1969) and have served as standard reference tables for inviscid flow about circular cones.

Finally some results are shown from MOL solutions for flow about the compression side of a delta wing at incidence to a supersonic stream. Again a comparison is made with a hyperbolic marching method.

Other nonlinear examples are discussed in Jones, South and Klunker (1972).

4.2 The Simply Supported Square Plate

For this example we use the following notation

C	constant = $tE/(1-\nu^2)$
D	flexural rigidity, $Et^3/12\,(1-\nu^2)$
E	modulus of elasticity, = 2×10^{10}
t	plate thickness, = 0.002
N	number of strips used. h = ½/N
p	= u_x
q	= v_x
Q	normal pressure. Varies from 0 to 80
r	= w_x
s	= α_x
u,v	mid plane displacements in x and y directions
w	transverse displacement
α	substituted for $w_{xx} + w_{yy}$
δx	step length used for integrating the MOL ordinary differential equations
h	strip width in y direction
ν	Poisson's ratio, = 0.3

The example is a structural problem which is defined mathematically by a set of rather complicated nonlinear partial differential equations. These are

$$u_{xx} + w_x w_{xx} + \nu(v_{xy} + w_y w_{xy}) + \tfrac{1}{2}(1-\nu)$$

$$\cdot(u_{yy} + v_{xy} + w_x w_{yy} + w_y w_{xy}) = 0 \tag{4.1a}$$

$$v_{yy} + w_y w_{yy} + \nu(u_{xy} + w_x w_{xy}) + \tfrac{1}{2}(1-\nu)$$

$$\cdot(v_{xx} + u_{xy} + w_y w_{xx} + w_x w_{xy}) = 0 \tag{4.1b}$$

$$D\nabla^4 w = Q + \frac{tE}{1-\nu^2}\left\{[u_x + \tfrac{1}{2}w_x^2 + \nu(v_y + \tfrac{1}{2}w_y^2)]\right.$$

$$\cdot w_{xx} + [v_y + \tfrac{1}{2}w_y^2 + \nu(u_x + \tfrac{1}{2}w_x^2)]\, w_{yy}$$

$$\left. + (1-\nu)(u_y + v_x + w_x w_y) w_{xy}\right\} \tag{4.1c}$$

subject to boundary conditions on the simply supported square plate $o \leqslant x \leqslant 1$, $o \leqslant y \leqslant 1$

$$x = o:\ u = v = w = w_{xx} = o \tag{4.2a}$$

$$y = o:\ u = v = w = w_{yy} = o \tag{4.2b}$$

with lines of symmetry $x = \tfrac{1}{2}$, $y = \tfrac{1}{2}$.

To use MOL, Equations (4.1) are written as differential equations of first order in x which is the variable to be left continuous. We also for convenience, introduce a variable $\alpha = \nabla^2 w$ (hence, on the boundaries, $\alpha = o$), and suitably scale the dependent variables $\bar{u} = Cu$, $\bar{v} = Cv$, $\bar{w} = C^{1/2}w$, $\bar{\alpha} = C^{1/2}\alpha$. Then, dropping the bar notation, the Equations (4.1) can be written as the system of equations

$$u_x = p \tag{4.3a}$$

$$v_x = q \tag{4.3b}$$

$$w_x = r \tag{4.3c}$$

$$\alpha_x = s \tag{4.3d}$$

$$r_x = \alpha - w_{yy} \tag{4.3e}$$

$$p_x = - [r r_x + \nu(q_y + w_y r_y) + \tfrac{1}{2}(1-\nu) \cdot (u_{yy} + q_y + r w_{yy} + w_y r_y)] \tag{4.3f}$$

$$q_x = - 2(1-\nu)^{-1} [v_{yy} + w_y w_{yy} + \nu(p_y + r r_y)] - p_y - w_y r_x - r r_y \tag{4.3g}$$

$$Ds_x = - D\alpha_{yy} + C^{\frac{1}{2}}Q + [p + \tfrac{1}{2} r^2 + \nu(v_y + \tfrac{1}{2} w_y^2)] r_x + [v_y + \tfrac{1}{2} w_y^2 + \nu(p + \tfrac{1}{2} r^2)] w_{yy} + (1-\nu)[u_y + q + r w_y] r_y \tag{4.3h}$$

Now Equations (4.3) are to be satisfied on each dividing line (except at y = o) which are numbered 0,1,2 . . . N say corresponding to increasing y. Thus $y_o = 0$, $y_N = \tfrac{1}{2}$ and the strip width $h = 1/2N$. Symmetry on $y = \tfrac{1}{2}$ can be conserved by introducing image lines at $\tfrac{1}{2} + h$ and $\tfrac{1}{2} + 2h$ and these lines are numbered N + 1 and N + 2. Then for symmetry

$$v_{N+k} = - v_{N-k}$$

$$q_{N+k} = - q_{N-k}$$

for k = 1,2 while for the other dependent variables the equality holds (e.g. $w_{N+k} = w_{N-k}$).

The partial derivatives with respect to y occurring in Equations (4.3) are replaced by the five line difference formulas (2.17) for i = 2,3 . . . N, while on line 1 we use formulas (2.19) and (2.20).

Now we can apply MOL by estimating p,q,r and s at each line i at x = o. These estimates are made by first obtaining a solution with Q near zero since at Q = 0 we know p = q = r = s = o. We then increase Q gradually and obtain initial estimates of p,q,r and s at x = o by extrapolation from previous solutions; in our case quadratic extrapolation was used as soon as possible. We then improve the estimates using Powell's method in order that

$$r^2 + q^2 + u^2 + s^2 \tag{4.4}$$

at each line at $x = \tfrac{1}{2}$ is minimized. The latter must be minimized since we require

$$r = q = u = s = o$$

at $x = \frac{1}{2}$ to preserve symmetry there. In the practical computation it turned out that weighting factors had to be applied in (4.4) so that each term was roughly of the same order.

The integration method used was Hamming's (1959) predictor modifier corrector scheme of $0(\delta x^5)$ accuracy. Starting with N = 3 various step lengths δx were used i.e. $\delta x = \frac{1}{2}/m$ where m = 3,4,5, 6,7,8,10. This procedure indicated the step length δx needed to give sufficient accuracy. It was found that $\delta x = 1/20$ was sufficiently small since these results differed only a little from $\delta x = 1/16$.

We then used N = 4 lines ($\delta x = 1/20$) and compared the results with N = 3 for Q = 32. Some quantities were not sufficiently accurate, e.g. w_{yy}, so we next used N = 5 and again compared results at Q = 32. Some of these comparisons are shown in Figures 4.1. It was found that, with N = 5, solutions were rather difficult to obtain for $Q > 32$; this was due to the instability becoming more significant as the nonlinearity of the problem increased (parallel shooting (Section 2.9) would have to be used to obtain solutions with higher Q). However using the one shooting range we obtained satisfactory results with N = 3 or 4. Solutions at Q = 80 are compared in Figures 4.2 with a 9 element finite element solution of Dixon (1971). It is seen that good agreement is obtained.

The time taken for the MOL solutions for some 40 values of Q between 0 and 80 was as follows

$$N = 3, \quad \delta x = \frac{1}{20}: \quad 2.5 \text{ mins.}$$

$$N = 4, \quad \delta x = \frac{1}{20}: \quad 3.5 \text{ mins.}$$

on an IBM 3032 computer.

4.3 Conical Flow Problems

The method of lines seems to be ideally suited to problems of this type since it is not clear how one would solve the **elliptic** system by finite difference methods. The previous finite difference methods (e.g. Babenko 1966) solved the **hyperbolic** system of equations by a marching technique using the cone axis z (see Fig. 4.3) as the time-like direction. But these marching methods were rather slow, for example, Gonidou (1969) reported one hour computation for a certain configuration and, as many solutions for different configurations were required, it seemed that a more efficient computational technique was needed. MOL turned out to be very efficient with between 5 and 20 seconds needed for a solution. For flows about circular cones a set of tables of MOL results has been published by Jones (1969); results for some 1200 configurations are listed there.

The physical problem is shown in Figure 4.3. In supersonic flow there is a shock wave attached to the tip of the conical body and the flow field behind the shock is such that quantities along any ray emanating from the tip are constant. We wish to find the shock wave shape and the flow field variables between the conical body in supersonic flow and its attached shock wave. A cylindrical co-ordinate system (z,r,θ) is adopted with the z axis along the axis of the conical body (which may for example be a circular cone).

The equation of the given body can be written in the form, $r = zG(\theta)$ say, and we let the equation of the unknown attached shock wave be $r = zF(\theta)$. The full three-dimensional equations of motion (momentum, continuity and energy conservation) can be written in matrix form as

$$A' \frac{\partial X}{\partial z} + B' \frac{\partial X}{\partial r} + C' \frac{\partial X}{\partial \theta} + D' = 0, \tag{4.5}$$

where $A'B'C'$ are (5×5) matrices, D' is a column vector and X is also a column vector given by

$$X = \begin{pmatrix} u \\ v \\ w \\ p \\ \rho \end{pmatrix},$$

where u,v,w are the velocity components in the (z,r,θ) directions, respectively, p is the pressure and ρ the density. The matrices and the vector D' consist of elements which are functions of u,v,w,p, and ρ; their exact form can be found in Jones (1968). A cross section (z = const) of the flow field is shown in Figure 4.4a; here the flow and body are assumed to be symmetrical about $\theta = 0, \pi$ as is usually the case. The boundary conditions to be satisfied are the Rankine-Hugoniot relations at the shock wave which can be written in the form

$$X = f(\alpha,\gamma,M_\infty,\theta,F,F'), \tag{4.6}$$

where f is a column vector whose elements are functions of the listed arguments. The first three arguments in (4.6) are α the angle of incidence which is the angle that the direction of the free stream makes with the z axis, γ the ratio of specific heats and M_∞ the free-stream Mach number. Since these three arguments are known for a given problem it follows that the elements of X are known at the shock once the equation of the shock $r = zF(\theta)$ is known. F' is found from (2.17a).

On the body the normal velocity should be zero and can be written

$$uG - v + (1/G)(dG/d\theta)w = 0. \tag{4.7}$$

Now it is known that the equations of motion (4.5) can be reduced to two dimensions since the flow is conical. A suitable transformation to do this and also one which makes the boundaries easier to handle is given by

$$x = z,$$

$$\xi = [r - zG(\theta)]/z[F(\theta) - G(\theta)],$$

$$\phi = \theta.$$

It is now seen that the body $r = zG(\theta)$ and shock wave $r = zF(\theta)$ are transformed to the lines $\xi = 0$ and $\xi = 1$, respectively, see Figure 4.4b. The equations of motion (4.5) are transformed to

$$B(\partial X/\partial \xi) + C(\partial X/\partial \phi) + D = 0, \tag{4.8}$$

where B,C are (5×5) matrices and D is a column vector. The term $\partial X/\partial x$ is omitted from the above equation since the flow is conical and $\partial X/\partial x$ is zero. Now we can consider the equations at unit distance $x = z = 1$. Hence the problem is reduced to that of finding solutions of (4.8) in the region

$0 \leqslant \xi \leqslant 1$, $0 \leqslant \phi \leqslant \pi$ (assuming symmetry) subject to boundary conditions (4.6) at $\xi = 1$ and (4.7) at $\xi = 0$.

The method of lines is applied in the (ξ,ϕ) plane; symmetry conditions at $\phi = 0$ and at $\phi = \pi$ are satisfied by introducing image lines in the usual manner. An estimate for $F(\phi)$ at each of the lines is made, $F'(\phi)$ is obtained from (2.17a) and substitution in (4.6) gives $X(\xi = 1)$. Equations (4.8) are next reduced to ordinary differential equations by writing $\partial X/\partial\phi$ at each line in the finite-difference form (2.17a). Integration of these ordinary differential equations is then made from $\xi = 1$ to $\xi = 0$ where Equation (4.7) must be satisfied at each dividing line. The shock shape, i.e., $F(\phi)$ is changed by Powell's method so that conditions (4.7) are satisfied to a required accuracy. It was found convenient in this example to represent $F(\phi)$ by a cosine Fourier series $\Sigma_{i=0}^{m} F_i \cos i\phi$, say, where m is 1 or 2 for the circular cone at small angles of incidence; by this representation the number of unknowns is reduced and so the work involved in finding the partial derivatives in (2.11) is reduced and also Powell's method is more efficient.

It is important in this example to have a good estimate of the shock shape $F(\phi)$. To be always sure of a good estimate, a situation is first considered for that of a circular cone $r = G(\phi) = \text{const}$ which is at incidence $\alpha = 0$ deg. For this case the flow is axisymmetric and the problem is easily solved. A situation is next considered which has a small perturbation from the circular cone at zero incidence [either a small change to the body shape $G(\phi)$ or a small change in incidence may be considered]. In this case the estimate for $F(\phi)$ is taken to be that obtained for the first case of the circular cone at zero incidence. The solution for this small perturbation is then found by the method of lines. Next a larger perturbation of body shape or incidence, which is proportional to the first perturbation, is considered and $F(\phi)$ is estimated by extrapolation from the two previous results. And so the technique can be continued for larger proportional perturbations and always a good estimate for $F(\phi)$ is available by extrapolation from previous results at the smaller perturbations. For example, to find solutions at incidence for the circular cone whose semi-apex angle is θ_c, a solution is first found for $\alpha = 0$ deg., then successively for $\alpha/\theta_c = 0.01, 0.1, 0.2, 0.3, \ldots$.

By the method of lines it was possible to generate solutions for the circular cone for relative incidence α/θ_c as high as 1.4 in some cases, which was higher than relative incidences at which any other theoretical solutions were available. The only other methods available which gave solutions at relative incidences greater than unity (up to about 1.2) are methods which solved the full hyperbolic Equations (4.5) [Babenko 1966, Gonidou 1968] and these methods are 50-100 times less efficient than the method of lines.

The quality of the results for a circular cone can be seen in Table VIII which compares surface values and shock shape $F(\phi)$ on a circular cone obtained by MOL with $\delta\phi = 22.5°$ and $\delta\xi = 0.1$ and by the method of Babenko et al. (1966) with $\delta\phi = 11.25$ and $\delta\xi = 0.05$, which solves the full hyperbolic Equations (4.5).

Results for a non circular cone are shown in Figure 4.5a and are compared with experimental results. The cross section of the body in this case is shown in Figure 4.5b.

Finally a surface pressure result of Klunker et al. (1971) for the delta wing problem (compression side) is given in Figure 4.6. In this problem, the cross section of the wing is flat, and the shock wave is attached not only at the wing apex, but also along the leading edges which are swept back 50°. The total velocity is everywhere supersonic, but in this problem the conical cross flow is also supersonic in a region adjacent to the leading edge ($\bar{x} = 1$ on Fig. 4.6). It is interesting that MOL can be used without difficulty in this case, even though the conical equations are of mixed type; MOL gives an excellent prediction of the constant pressure which occurs in the hyperbolic region (for the flat wing) as well as in the elliptic region near the wing center line ($\bar{x} = 0$ on Fig. 4.6), where the cross flow is conically subsonic. In Figure 4.6 the MOL results are compared with those of Voskresenskii (1968), who used the three-dimensional, fully hyperbolic, finite-difference method. It can be seen that the two methods agree well, and that remarkable accuracy is obtained by MOL with only one intermediate line between the wing center line and leading edge (i.e., N = 2). Further MOL results for delta wing problems are given in Klunker et al. (1971), including comparisons with experiment and other calculative methods.

It may be noted in Figure 4.6 that Klunker et al. in applying MOL to the delta wing problem, did not use constant strip widths but took more lines in the region where there is more variation in quantities, i.e., near $\bar{x} = 0$ in Figure 4.6. This is possible in their case since they approximate derivatives by fitting a fourth-order polynomial to five adjacent points near to the point at which the derivative is required.

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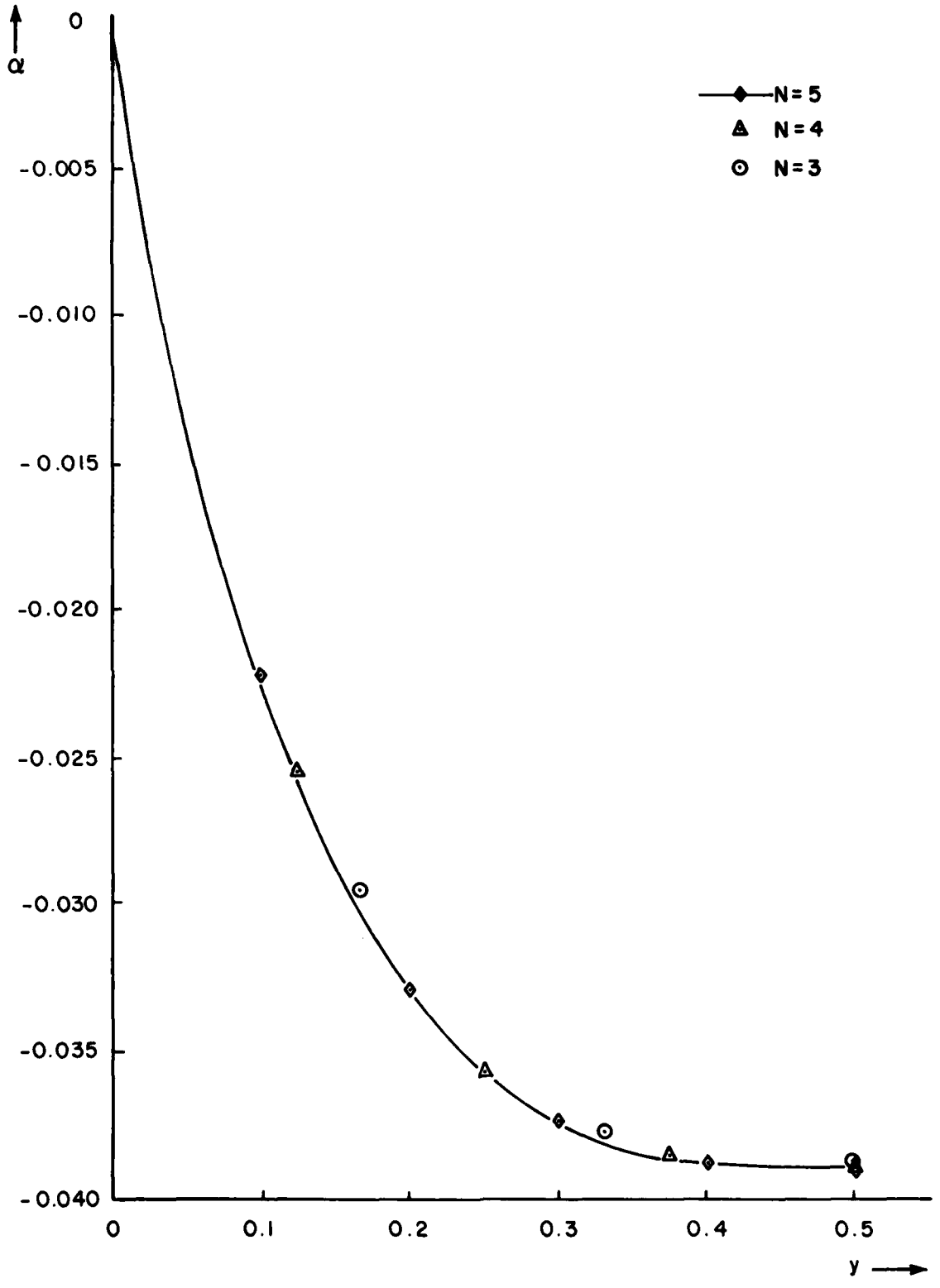


FIG. 4.1a STRUCTURES PROBLEM, SECTION 4.2. CONVERGENCE AS $\delta y \to o$. $x = 0.5$, $\delta x = 1/20$, $Q = 32$.

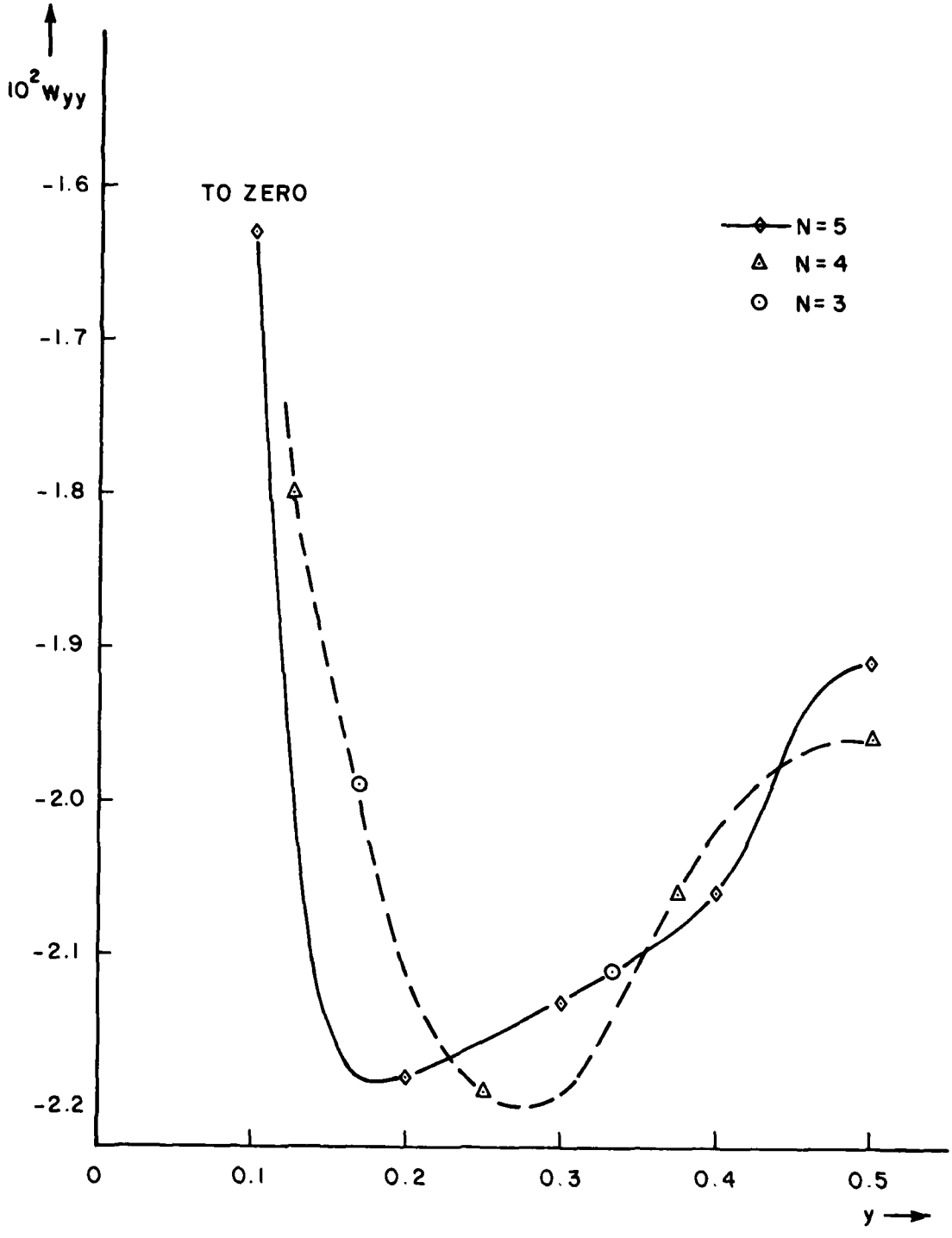


FIG. 4.1b STRUCTURES PROBLEM, SECTION 4.2. CONVERGENCE AS $\delta y \to o$. $x = 0.5$, $\delta x = 1/20$, $Q = 32$.

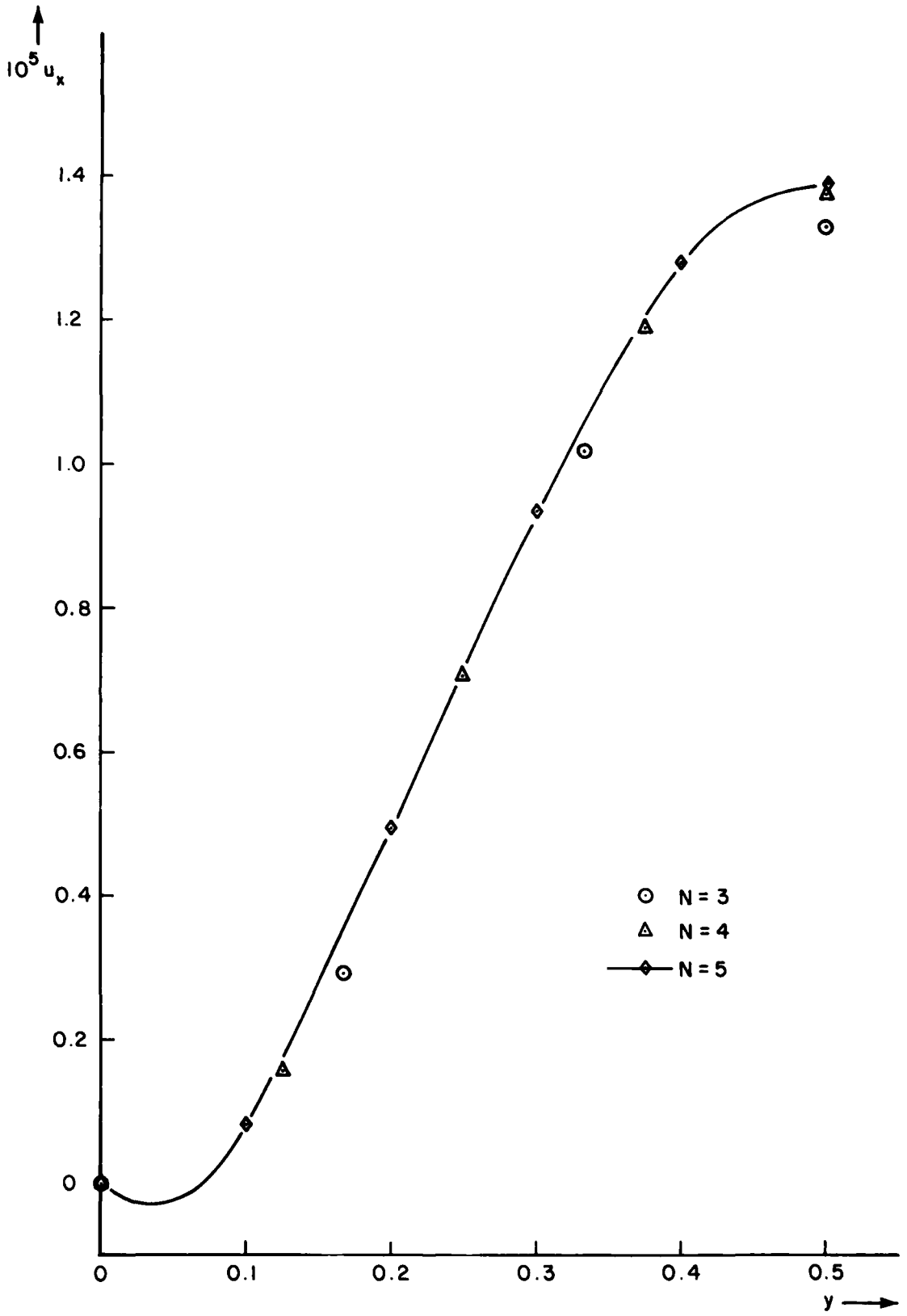


FIG. 4.1c STRUCTURES PROBLEM, SECTION 4.2. CONVERGENCE AS $\delta y \to o$. $x = 0.5$, $\delta x = 1/20$, $Q = 32$.

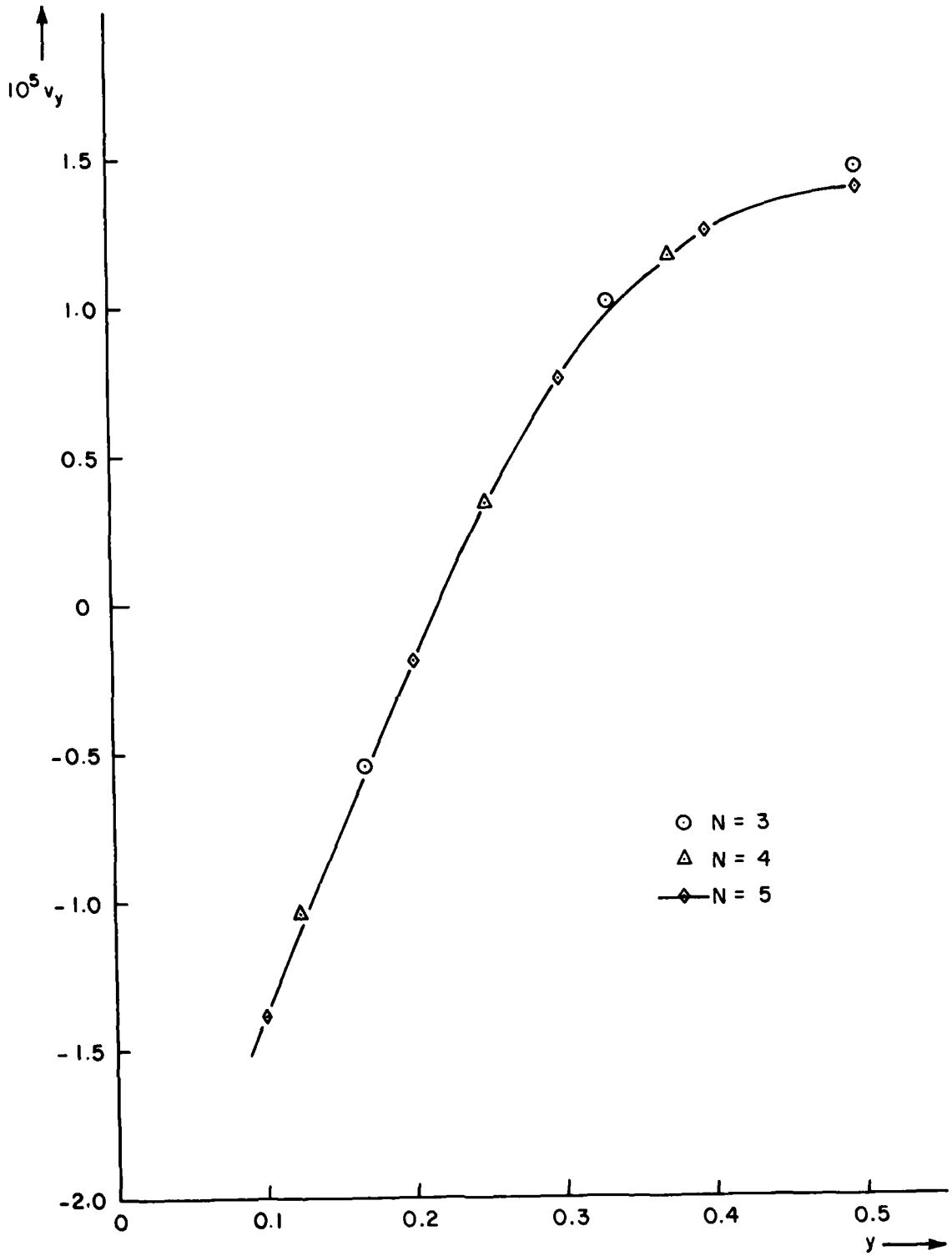


FIG. 4.1d STRUCTURES PROBLEM, SECTION 4.2. CONVERGENCE AS $\delta y \to o$. $x = 0.5$, $\delta x = 1/20$, $Q = 32$.

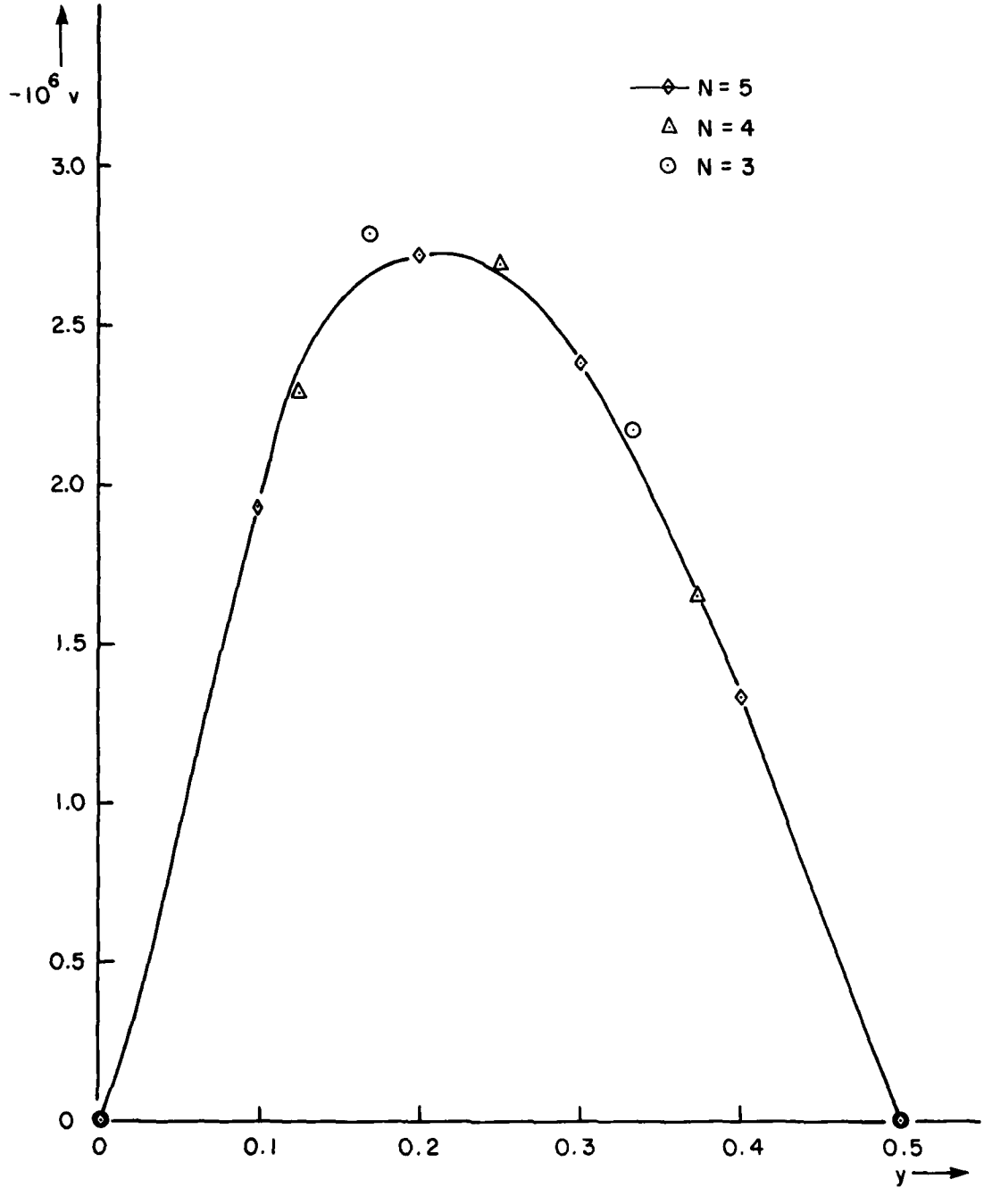


FIG. 4.1e STRUCTURES PROBLEM, SECTION 4.2. CONVERGENCE AS $\delta y \to o$. $x = 0.5$, $\delta x = 1/20$, $Q = 32$.

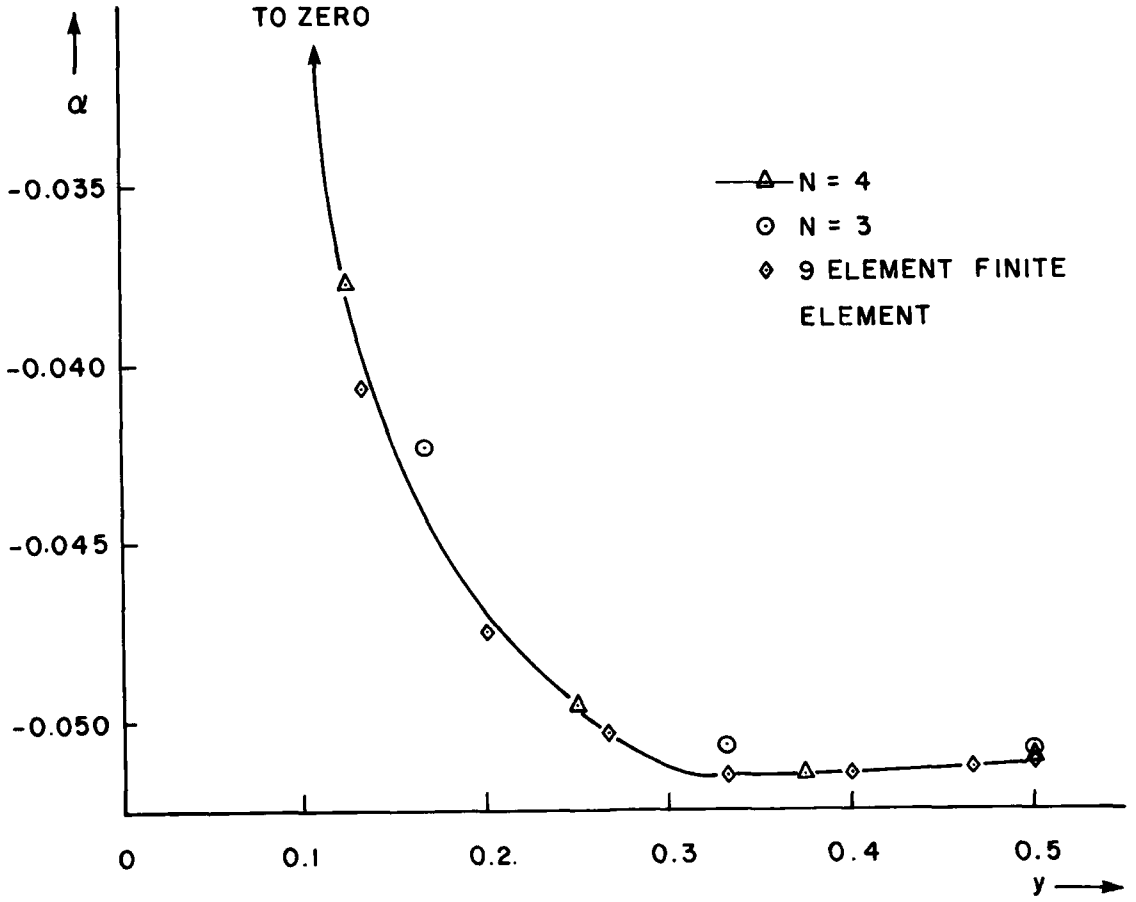


FIG. 4.2a COMPARISON OF RESULTS USING N = 3 AND N = 4 WITH FINITE ELEMENTS. x = 0.5, δx = 1/20, Q = 80.

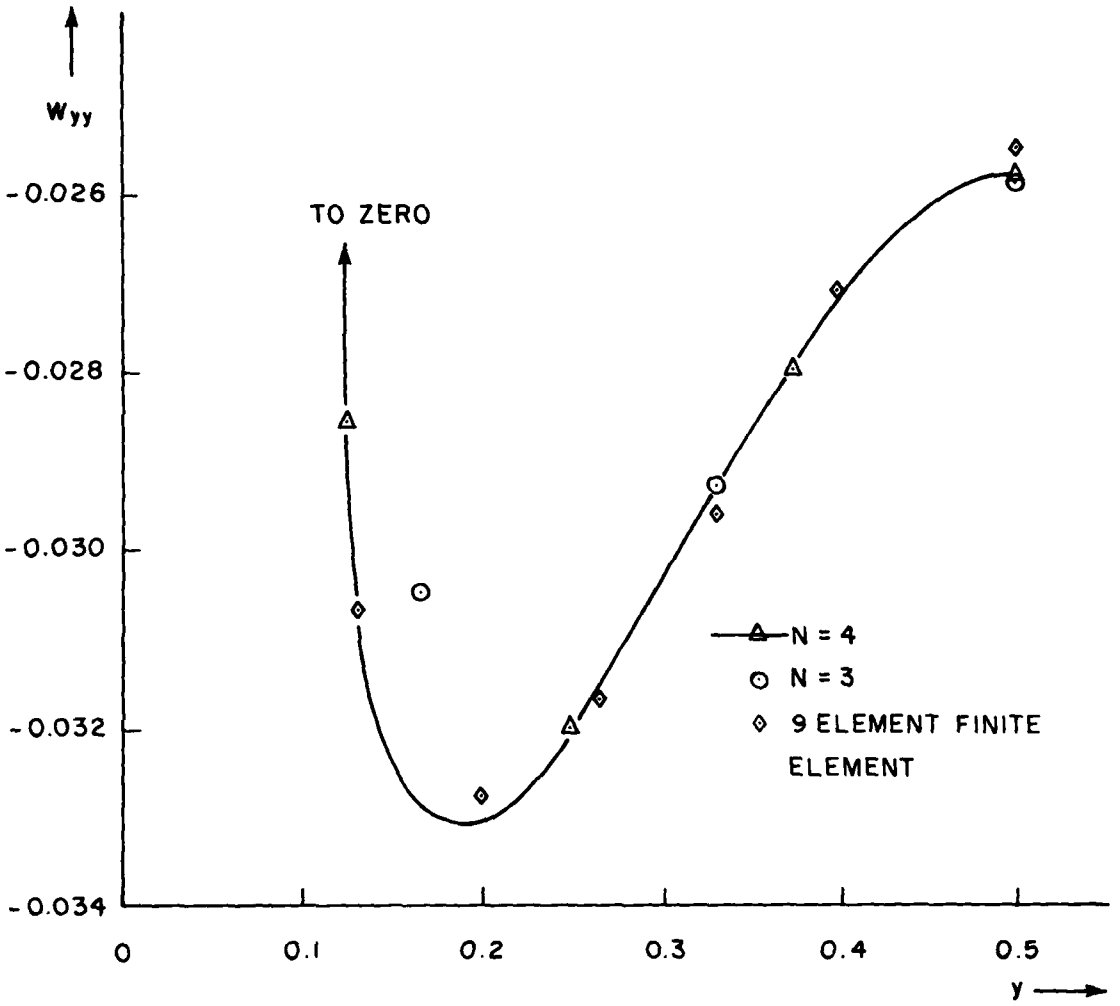


FIG. 4.2b COMPARISON OF RESULTS USING N = 3 AND N = 4 WITH FINITE ELEMENTS. $x = 0.5$, $\delta x = 1/20$, $Q = 80$.

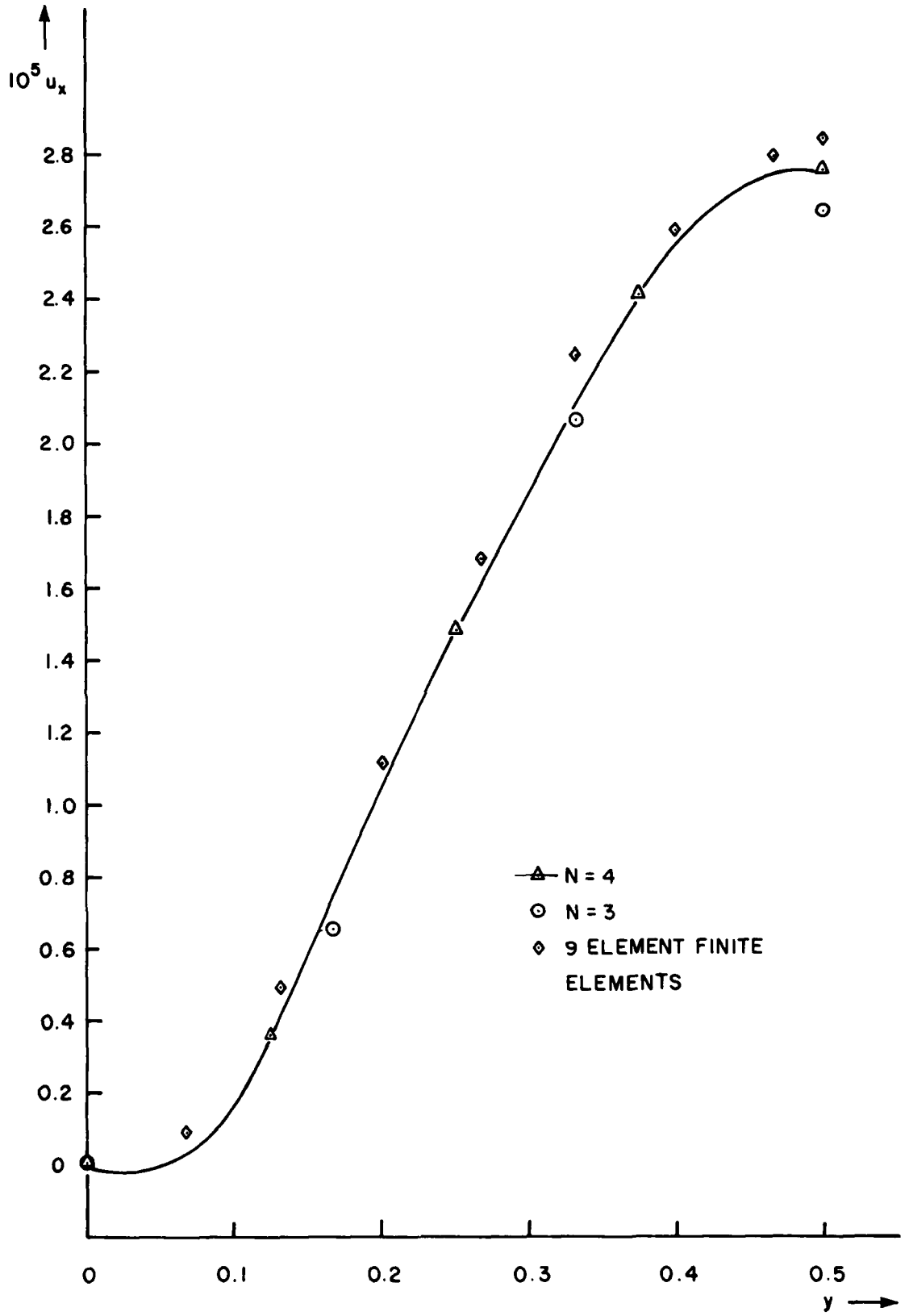


FIG. 4.2c COMPARISON OF RESULTS USING N = 3 AND N = 4 WITH FINITE ELEMENTS. x = 0.5, δx = 1/20, Q = 80.

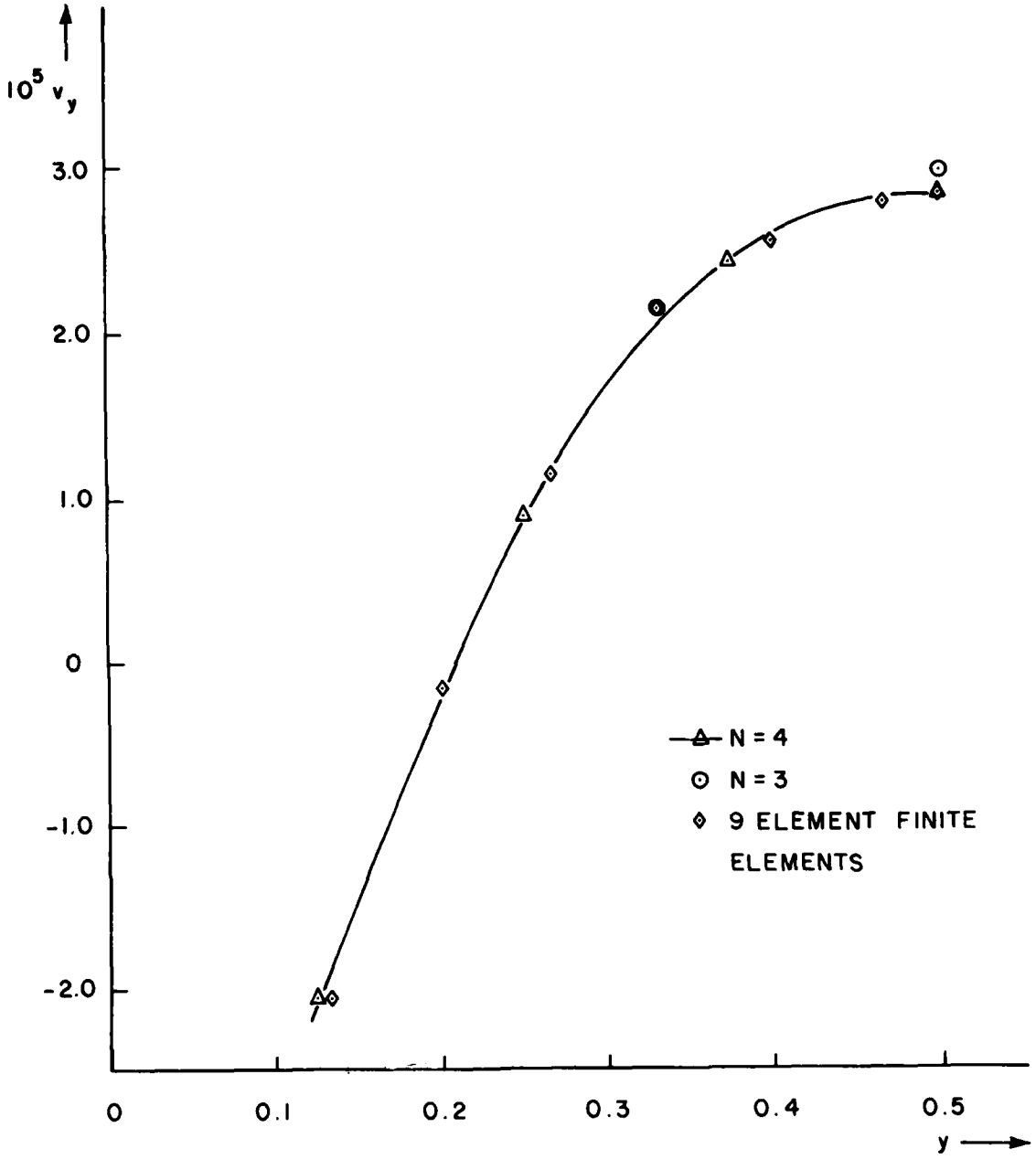


FIG. 4.2d COMPARISON OF RESULTS USING N = 3 AND N = 4 WITH FINITE ELEMENTS. x = 0.5, δx = 1/20, Q = 80.

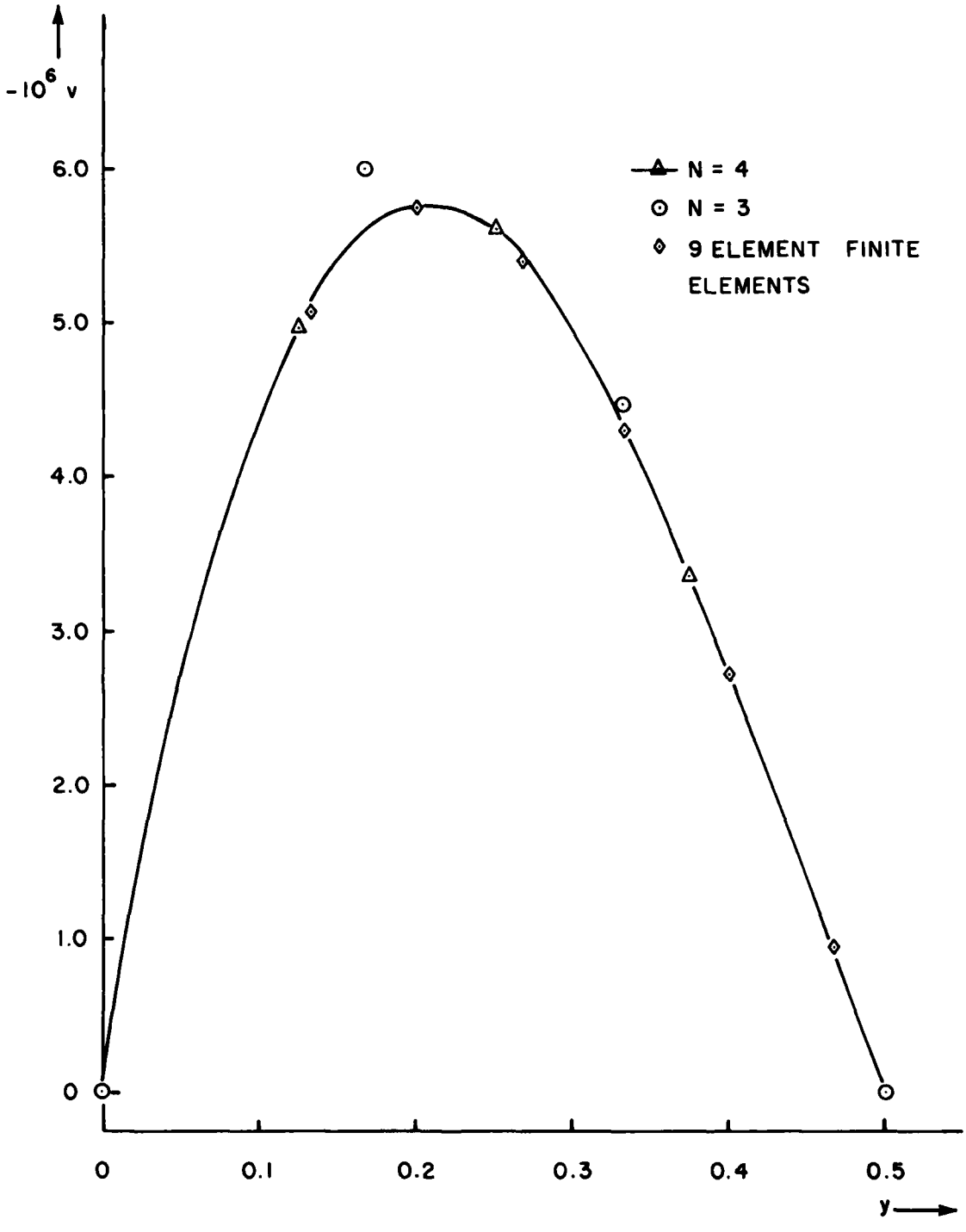


FIG. 4.2e COMPARISON OF RESULTS USING N = 3 AND N = 4 WITH FINITE ELEMENTS. x = 0.5, δx = 1/20, Q = 80.

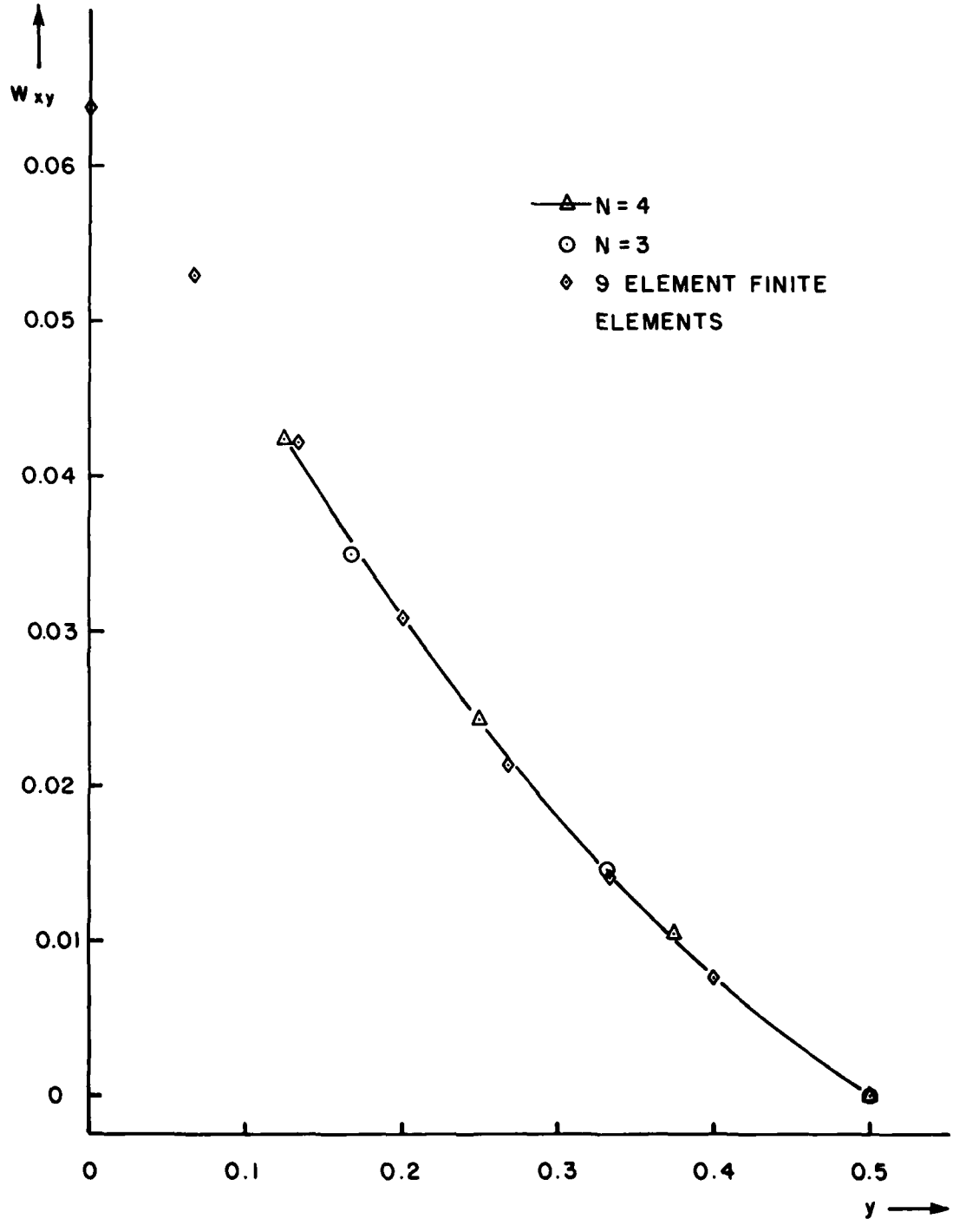


FIG. 4.2f COMPARISON OF RESULTS USING N = 3 AND N = 4 WITH FINITE ELEMENTS. x = 0.5, δx = 1/20, Q = 80.

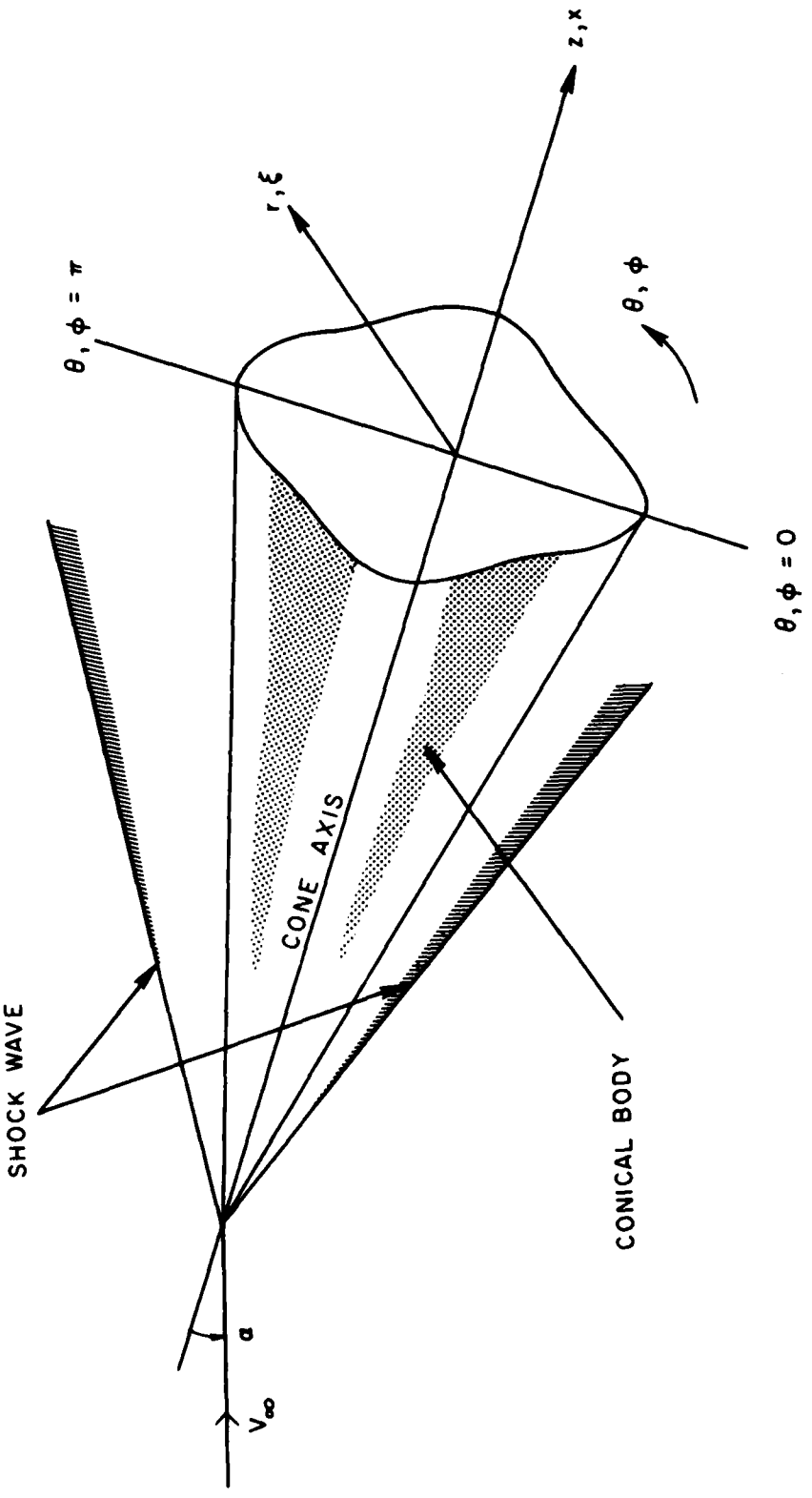
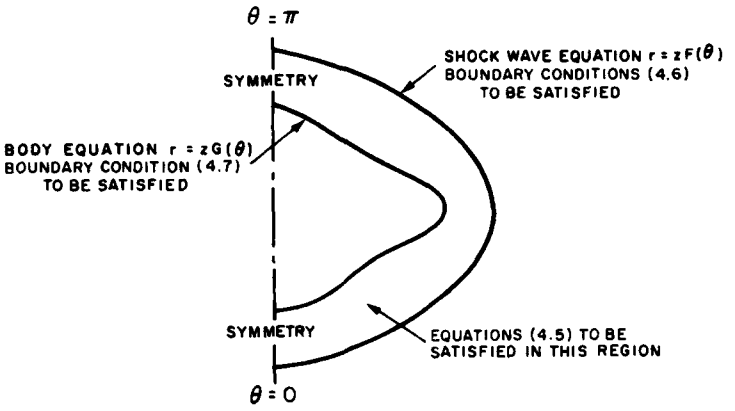


FIG. 4.3 CONICAL FLOW PROBLEM



BOUNDARIES ARE TRANSFORMED TO A SIMPLER FORM BY THE TRANSFORMATION

$$x = z$$

$$\xi = \frac{r - z\,G(\theta)}{z[F(\theta) - G(\theta)]}$$

$$\phi = \theta$$

GIVING THE REGION IN FIG. 4.4b

FIG. 4.4a CROSS SECTION z = CONSTANT OF THE FLOW FIELD; CONICAL FLOW PROBLEM

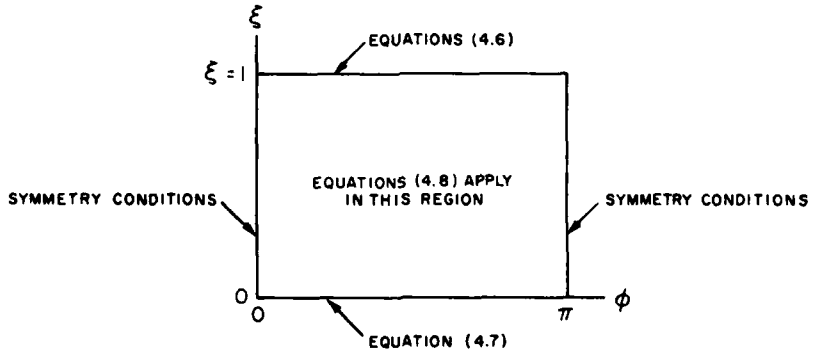


FIG. 4.4b

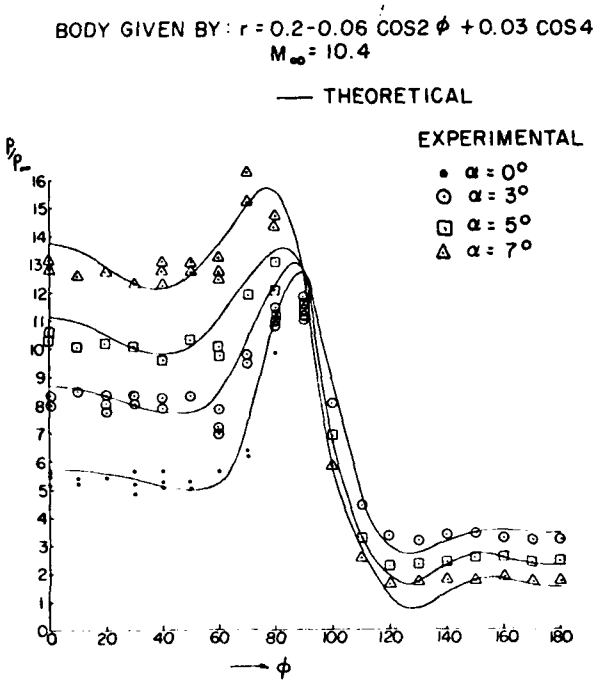


FIG. 4.5a COMPARISONS OF EXPERIMENTAL AND THEORETICAL PRESSURE DISTRIBUTIONS FOR BODY GIVEN BY FOURTH ORDER EVEN COSINE FOURIER SERIES

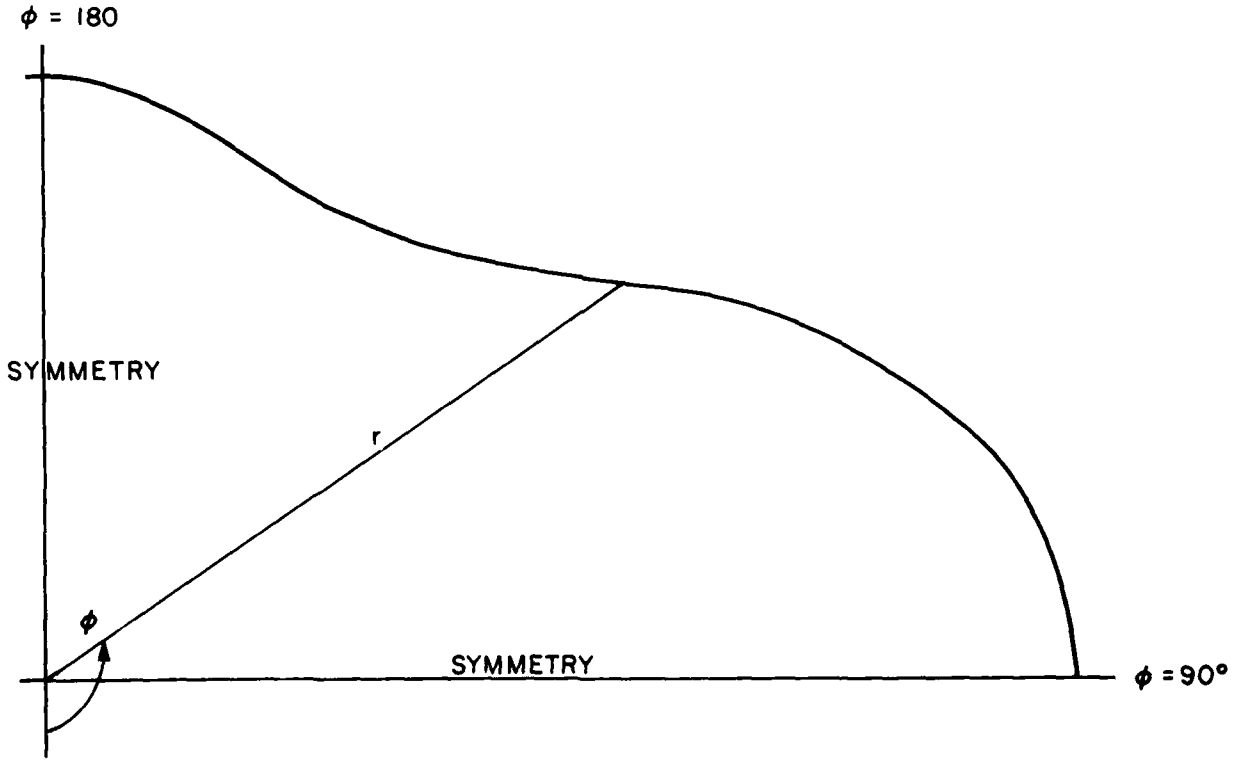


FIG. 4.5b BODY SHAPE USED IN CONICAL FLOW PROBLEM

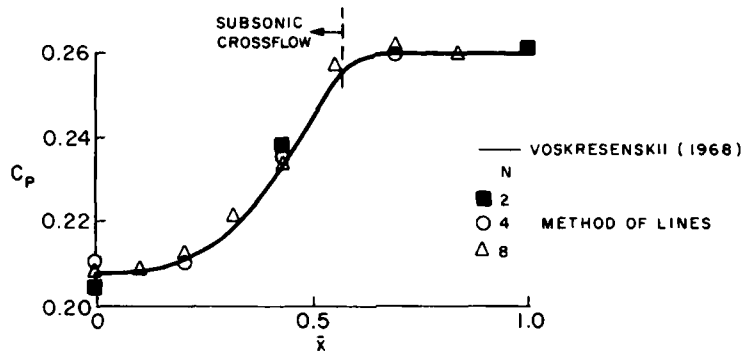


FIG. 4.6 SURFACE PRESSURE ON FLAT DELTA WING, $M_\infty = 4.0$, $\Lambda = 50°$, $\alpha = 15°$; MOL AND FINITE-DIFFERENCE HYPERBOLIC SOLUTIONS

TABLE VIII

COMPARISONS OF SURFACE VALUES AND SHOCK SHAPE BETWEEN PRESENT THEORY AND THE THEORY OF BABENKO ET AL. (1966) FOR CIRCULAR CONE

$M_\infty = 5, \quad \theta_c = 25, \quad \alpha = 20$

ϕ	0	22.5	45	67.5	90	112.5	135	157.5	180
u_J	1.3028	1.3167	1.3571	1.4205	1.5026	1.5956	1.6906	1.7741	1.8123
u_B	1.3026	1.3165	1.3572	1.4217	1.5048	1.5989	1.6936	1.7711	1.8129
v_J	0.6075	0.6140	0.6328	0.6624	0.7007	0.7440	0.7883	0.8273	0.8451
v_B	0.6074	0.6139	0.6329	0.6630	0.7017	0.7456	0.7897	0.8259	0.8454
w_J	0	0.1785	0.3464	0.4862	0.5890	0.6358	0.6205	0.4319	0
w_B	0	0.1792	0.3446	0.4832	0.5818	0.6285	0.6075	0.4463	0
p_J	2.6838	2.5058	2.0418	1.4619	0.9277	0.5447	0.3172	0.2426	0.2522
p_B	2.6842	2.5062	2.0423	1.4596	0.9282	0.5434	0.3182	0.2436	0.2508
ρ_J	4.7758	4.5474	3.9284	3.0946	2.2362	1.5288	1.0391	0.8580	0.8819
ρ_B	4.7759	4.5475	3.9289	3.0909	2.2368	1.5260	1.0411	0.8603	0.8785
F_J	0.5919	0.5943	0.6029	0.6168	0.6395	0.6657	0.6960	0.7075	0.6920
F_B	0.5920	0.5947	0.6028	0.6173	0.6388	0.6665	0.6949	0.7068	0.6917

Subscripts: J Values obtained by present method

B Values obtained by Babenko et al. (1966)

CHAPTER 5.0 ELLIPTIC EIGENVALUE PROBLEMS

5.1 Introduction

Although the main advantage of the method of lines has been in solving boundary value problems, particularly the rather complicated nonlinear types mentioned in Chapter 4, we feel that for completeness some coverage should be given to eigenvalue problems. Thus in this chapter we consider the method of lines solution to Helmholtz equation in a rectangle and compare MOL results to the exact solution.

The instability problems mentioned earlier (Section 3.3) are again encountered in the eigenvalue case. However it is illustrated that accurate results can be obtained for the smaller eigenvalues using the usual five line difference scheme (2.17). We first consider the three line scheme as this gives better insight into the stability and accuracy expected.

The problem considered here has a linear operator but nonlinear operators would be handled in a similar manner.

5.2 The Method of Lines Applied to Eigenvalue Problems

Consider Helmholtz' equation in a rectangle $o \leqslant x \leqslant a$, $o \leqslant y \leqslant b$. Lines are drawn parallel to the x axis and numbered 0, 1, ... N. Because of symmetry we consider only the region $o \leqslant x \leqslant a/2$, $o \leqslant y \leqslant b/2$. Lines o, N correspond to $y = 0$ and $y = b/2$ respectively. Writing $h = b/2N$ and replacing $\partial^2\psi/\partial y^2$ on the nth line by the three line finite difference scheme (2.5), for example, we have

$$\frac{dp_n}{dx} + \frac{\psi_{n+1} - 2\psi_n + \psi_{n-1}}{h^2} + k^2\psi_n = 0 \qquad (5.1a)$$

where

$$\frac{d\psi_n}{dx} = p_n \qquad n = 1,2 \ldots N \qquad (5.1b)$$

We apply symmetry at $y = b/2$ by making $\psi_{N+1} = \psi_{N-1}$. The initial conditions at $x = 0$ are

$$\psi_n = 0 \qquad n = 1,2 \ldots N$$

We can integrate (5.1) from $x = 0$ to $x = a/2$ provided we have values for k and for the gradients p_n for $n = 2,3 \ldots N$. The gradient p_1 is kept fixed throughout since we want to avoid the trivial solution $\psi = 0$. Note that this fixing of a gradient $\neq 0$ may prevent finding the eigenvalue corresponding to an eigenvector which has zero gradient at that point. For example if we fixed $p_{N-1} \neq 0$ when $N = 3$ then we could not calculate the eigenvalue corresponding to

$$\psi = A \sin\frac{m\pi x}{a} \sin\frac{3\pi y}{b}$$

since

$$\frac{d\psi_n(x = 0)}{dx} = A\frac{m\pi}{a}\sin\frac{3\pi y_n}{b} = \frac{Am\pi}{a}\sin\frac{3\pi(N - 1)h}{Nh} = 0$$

when N = 3. By increasing N to 4,5 . . . . , though, we could calculate the eigenvalue. Choosing $p_1 \neq 0$ for this particular problem does not lead to any eigenvalue loss.

Since the problem is linear for a fixed k we proceed as follows. Fix k in an outer loop. In the inner loop calculate $p_2 \ldots . p_N$ so that the sum of squares of residuals $\sum_{i=1}^{N} r_i^2 \left[\equiv \sum_{i=1}^{N} p_i^2\right]$ at x = a/2 is minimized. The generalized least squares minimization leads to

$$\sum_{j=2}^{N}\left\{\sum_{k=1}^{N}\frac{\partial r_k}{\partial F_i}\frac{\partial r_k}{\partial F_j}\right\}\delta F_j = -\sum_{k=1}^{N} r_k\frac{\partial r_k}{\partial F_i} \qquad i = 2, \ldots . N \tag{5.2}$$

where $F_j \equiv p_j$ (x = 0) and δF_j is the change to be made in F_j so that Σr_i^2 is minimized. Since r_k is linear with respect to $(F_2 \ldots . F_N)$, (5.2) is exact and the partial derivatives can be found exactly (within round off errors) by differences

$$\frac{\partial r_k}{\partial F_i} = \frac{r_k(F_2 \ldots, F_i + \Delta F_i, \ldots F_N) - r_k(F_2 \ldots, F_i, \ldots F_N)}{\Delta F_i} \tag{5.3}$$

where ΔF_i is theoretically any value but the authors usually select $10^{-6}F_i$ if $F_i \neq 0$ since a large disturbance to F_i may prevent integration to x = a/2 to find r_k. Also if the operator is non linear then (5.3) is a good approximation only if ΔF_i is small. The first estimate of (F_i) is not too critical since the above method theoretically yields the exact minimum in the inner loop. However we have to select values which enable us to integrate to x = a/2 without the solution blowing up. In the example of this chapter we consistently set $F_1 = F_2 = \ldots . F_N = 1$ at the start of the inner loop, used $\Delta F_i = 10^{-6}F_i$, and did not encounter any difficulties. F_1 was then kept fixed on 1 and integrations made using the small perturbations to $F_2 \ldots . F_N$ in turn. Having found the partial derivatives according to (5.3) we then substitute into (5.2) and by Gaussian elimination find δF_j.

In the outer, k, loop we can either select values for k^2 in some consistent manner,

$$k^2 = c(d)e \tag{5.4}$$

say, or we can carry out a one dimensional minimization. The method used by the authors is a combination of both these possibilities. First c and e are selected (for example we chose c = 0, e = 65 in the square membrane problem to follow) and the step d is selected in a manner depending on the problem at hand (for the square membrane we chose d = 1 since we knew there were many roots expected in the range $o \leqslant k^2 \leqslant 65$). For a particular N we then plot R $(\equiv (\Sigma r_i^2)^{1/2})$ against k^2. The function R will have a cusp at each root (Fig. 5.1 for example) thus giving approximations $k_1^2, k_2^2 \ldots .$ to the eigenvalues. We may then, if required, calculate the roots more accurately by minimizing Σr_i^2 with respect to λ where λ is given by

$$k_i^2 = \tfrac{1}{2}(k_{i1}^2 + k_{io}^2) + \tfrac{1}{2}(k_{i1}^2 - k_{io}^2)\sin\lambda \qquad (5.5)$$

and k_i^2 is the ith eigenvalue. k_{io}^2 and k_{i1}^2 are lower and upper limits on k_i^2 chosen from the graphical inspection above. The authors preferred this semi-automatic method but a completely automated method could be devised in which the computer would locate each root approximately and then refine the approximation.

If we suspect the presence of multiple roots which numerically are roots which may be very close but not coincident we can then minimize

$$\sum_j r_j^2/(k_i^2 - k_{iA}^2)^2 \qquad (5.6)$$

in the ranges $k_{io}^2 \leqslant k_i^2 < k_{iA}^2$ and $k_{iA}^2 < k_i^2 \leqslant k_{i1}^2$ where k_{iA}^2 is the eigenvalue already found. Triple roots can be found in a similar manner.

The method has been described above using a three point approximation to the derivative ψ_{yy}. But in order to use as few lines as possible it is better to use finite difference approximations having greater accuracy. Application in this case is exactly the same as outlined above.

We next apply the method to a square membrane using the three point scheme (for which an analytical solution is available) and then use a five point scheme for which a semi-analytical solution is available.

5.3 Helmholtz' Equation in a Square

To investigate the accuracy, stability and convergence of MOL we consider a simple example with a known solution and solve the MOL ordinary differential equations first analytically and later numerically.

5.3.1 The Three Line Scheme

We consider a square of side π in which we want to solve $(\nabla^2 + k^2)\psi = 0$ subject to $\psi = 0$ on the boundary. The MOL representation of Helmholtz' equation using the three line scheme can be written

$$\psi_n'' + \frac{\psi_{n+1} - 2\psi_n + \psi_{n-1}}{h^2} + k^2\psi_n = 0 \qquad (n = 1,2 \ldots N) \qquad (5.7)$$

where $h = \pi/2N$ and lines are considered parallel to the x axis. Lines o, N are equivalent to $y = 0$ and $y = \pi/2$ respectively. The primes denote differentiation with respect to x. We consider only the region $o \leqslant x \leqslant \pi/2$, $o \leqslant y \leqslant \pi/2$ because of symmetry (or antisymmetry).

The boundary conditions are

$$x = 0: \quad \psi_n = 0 \qquad (n = 1,2 \ldots N) \qquad (5.8a)$$

$$x = \frac{\pi}{2}: \quad \psi_n' = 0 \quad \text{for symmetry} \qquad (n = 1,2 \ldots N)$$

$$[\text{or } \psi_n = 0 \quad \text{for antisymmetry}] \tag{5.8b}$$

$$\psi_{N+1} = \psi_{N-1} \quad \text{for symmetry}$$

$$[\text{or } \psi_{N+1} = - \psi_{N-1} \quad \text{for antisymmetry}] \tag{5.8c}$$

$$\psi_o = 0 \tag{5.8d}$$

It can be shown that the general solution to (5.7) subject to the boundary conditions (5.8c) and (5.8d) is

$$\psi_n = \sum_{m=1,3,5\ldots}^{2N-1} \sin \frac{nm\pi}{2N} \left[A_m \sin \mu_m x + B_m \cos \mu_m x\right] \tag{5.9}$$

where $\mu_m^2 = k^2 - (4/h^2) \sin^2 m\pi/4N$. Since the solution is real it follows that A_m is imaginary if $k < (2/h) \sin m\pi/4N$. We now apply the remaining boundary conditions (5.8a) and (5.8b) giving

$$\sum_m \sin \frac{nm\pi}{2N} B_m = 0 \qquad (n = 1,2 \ldots N) \tag{5.10a}$$

and

$$\sum_m \mu_m \sin \frac{nm\pi}{2N} \left[A_m \cos \frac{\mu_m \pi}{2} - B_m \sin \frac{\mu_m \pi}{2}\right] = 0 \qquad (n = 1,2 \ldots N) \tag{5.10b}$$

The system (5.10a), assuming that $\det(a_{n\ell}) \neq 0$ where $a_{n\ell} = \sin n(2\ell-1)\pi/2N$, shows that $B_1 = B_3 = \ldots = B_{2N-1} = 0$ and the system (5.10b) becomes

$$\sum_m \sin \frac{nm\pi}{2N} \cos \frac{\mu_m \pi}{2} \mu_m A_m = 0 \tag{5.10c}$$

For a non trivial solution we require $\mu_m A_m \neq 0$ for some m (see Equation (5.9)) and hence require the determinant of system (5.10c) to be zero i.e.

$$\prod_{m=1,3,5\ldots}^{2N-1} \cos \mu_m \frac{\pi}{2} \quad (\det a_{n\ell}) = 0$$

or since we assume $\det(a_{n\ell}) \neq 0$

$$\cos \mu_m \frac{\pi}{2} = 0 \qquad \text{for } m = 1,3 \ldots . \text{ or } 2N-1 \tag{5.11}$$

and so $\mu_m = p$ where p is one of the integers 1, 3, 5 .... Thus

$$k^2 = p^2 + \frac{4}{h^2} \sin^2 \frac{m\pi}{4N} \qquad \begin{matrix} p = 1,3,5 \ldots \\ m = 1,3, \ldots 2N-1 \end{matrix} \tag{5.12}$$

giving the MOL analytical approximation to the exact eigenvalues which in the symmetrical case are

$$k^2 = p^2 + m^2 \qquad \begin{matrix} p = 1,3,5 \ldots \\ m = 1,3,5 \ldots \end{matrix} \tag{5.13}$$

Since $h = \pi/2N$ the difference is

$$m^2 - \frac{16N^2}{\pi^2} \left[\frac{m^2\pi^2}{16N^2} - \frac{m^4\pi^4}{768N^4} + \ldots \right] = \frac{m^4\pi^2}{48N^2} + 0(N^{-4}) \tag{5.14}$$

indicating accuracy of $0(h^2)$ as expected. It can be seen from (5.14) that for the smallest eigenvalue (m = 1) the error will be $< 10^{-3}$ if $N > 15$. For m = 3 using the same number of lines the error would increase by a factor 81 and higher eigenvalues would rapidly increase in error. Values of k^2-p^2 found from the three point scheme, formula (5.12), are listed in Table IXa for N = 3,4,5,6,7 and 8. This table illustrates that accuracy for m = 1 is fairly good when N = 8 but that higher eigenvalues are poorly approximated.

The conclusion of this subsection is that many lines have to be used with the three point scheme in order to obtain a reasonable accuracy even for the smallest eigenvalue. Using such a large number of lines would undoubtedly lead to a large instability when applying MOL numerically and so we seek a difference scheme which is more accurate than the three line scheme. This will enable us to use fewer lines and so help to minimize the effect of the instability. In the next section we next consider such a scheme.

Note that the eigenvector for the three point scheme is

$$\psi_n = A \sin px \sin \frac{nm\pi}{2N} = A \sin px \sin my_n$$

which is exact in this case.

5.3.2 The Five Line Scheme

In this case ψ_{yy} in Helmholtz' equation is replaced by formula (2.17b) on interior lines and by formula (2.20) on the line adjacent to y = 0. As with the three line scheme the resulting problem of finding the eigenvalues can be reduced to finding the eigenvalues of a matrix. However these cannot be found in closed form as before but are found numerically.

Applying the five line scheme to Helmholtz' equation results in a set of ordinary differential equations of second order in x written at each line 1,2 . . . . N. On seeking a solution of the type $\psi_n = a_n \sin px$ we have

$$\frac{h^2}{2}(k^2 - p^2)a_1 - \frac{a_2 - a_1}{6} + \frac{1.75}{3}(a_3 - a_1) - \tfrac{1}{4}(a_4 - a_1)$$

$$+ \frac{0.125}{3}(a_5 - a_1) + \frac{1.25}{3}(a_0 - a_1) = 0 \qquad (5.15a)$$

$$h^2(k^2 - p^2)a_n + \frac{4}{3}(a_{n+1} + a_{n-1} - 2a_n) - \frac{1}{12}(a_{n+2} + a_{n-2} - 2a_n) = 0$$

$$n = 2,3 \ldots N \qquad (5.15b)$$

with boundary values $a_o = 0$, $a_{N+1} = a_{N-1}$ and $a_{N+2} = a_{N-2}$ for symmetry. To give a non trivial solution the determinant of the matrix of system (5.15) should be zero. For example using N = 3 we require

$$\det \begin{bmatrix} T - \frac{7}{6} & -\frac{5}{6} & \frac{3.5}{3} \\ \frac{4}{3} & T - \frac{31}{12} & \frac{4}{3} \\ -\frac{1}{6} & \frac{8}{3} & T - \frac{5}{2} \end{bmatrix} = 0$$

where $T = h^2(k^2 - p^2)$ i.e. we require the eigenvalues of the above matrix written without T on the main diagonal. If $\lambda_1, \lambda_2 \ldots . \lambda_N$ are the resulting eigenvalues then

$$k^2 - p^2 = -\frac{\lambda_i}{h^2} \qquad i = 1,2 \ldots N \qquad (5.16)$$

Now p = 1,3,5 . . . . to satisfy the boundary conditions $\psi_n = 0$ at x = 0 and ψ_n symmetrical about $x = \pi/2$. Thus the eigenvalues k^2 are determined from (5.16). Values of k^2-p^2 from Equation (5.16) are listed in Table IXb for N = 3,4,5,6,7 and 8. This table illustrates the accuracy to be expected from the five line scheme since the exact k^2-p^2 should be equal to m^2 for m = 1,3, ... 2N-1. The accuracy of the eigenvalues corresponding to m = 1 and 3 is very good while the m = 5 and 7 eigenvalues have about 1% accuracy at N = 8. Higher eigenvalues are poorly predicted. Note that convergence is rapid, for example the errors for the m = 5 eigenvalue are about 30%, 5%, 3%, 1.5% and 0.8% with N = 4,5,6,7 and 8 respectively. This feature is to be expected since the error is $0(N^{-4})$.

To compare the above MOL results with those obtained by finite differences we can use the formula given in Isaacson and Keller (1966) for the finite difference solution of accuracy $0(h^2)$ using an N × N mesh on a quarter of the square of side π i.e.

$$k^2 = \frac{16N^2}{\pi^2}\left[\sin^2\frac{p\pi}{4N} + \sin^2\frac{m\pi}{4N}\right]$$

c.f. Equation (5.12). For example, to achieve 1% accuracy for the eigenvalue corresponding to m = 5 and p = 1 would require a 22 × 22 mesh.

5.3.3 Numerical Solution by the Five Line Scheme

The three line and five line schemes, solved analytically above, illustrate the accuracy one might expect to obtain using MOL. We now proceed to the numerical procedure for solving the equations and use the five line scheme. But first we inspect the numerical instability which is similar to the instability encountered in boundary value problems (see Section 3.3).

As can be seen from the three line analytic solution (5.9, 5.10) we should have $B_m = 0$ and $A_m = 0$ except for the one A, say a, corresponding to $\mu_m = p$ i.e.

$$\psi_n = a \sin\frac{nm\pi}{2N} \sin px$$

is the exact solution for three point difference scheme. However numerically, since we treat the problem as an initial value problem, we will not have **exactly** $B_m = 0$ and $A_m = 0$. Instead these will take on small values perhaps of order 10^{-10}. And so, unwanted terms in expression (5.9) for ψ_n will be present and cause the inherent instability. This is likely to be significant if $k < (4N/\pi) \sin m\pi/4N$ since then there is a term present in (5.9) containing the factor

$$\sinh\left[\frac{16N^2}{\pi^2}\sin^2\frac{m\pi}{4N} - k^2\right]^{\frac{1}{2}} x$$

which for m = 2N-1 is

$$\sinh\left[\frac{16N^2}{\pi^2}\cos^2\frac{\pi}{4N} - k^2\right]^{\frac{1}{2}} x \simeq \sinh\left[\frac{16N^2}{\pi^2} - k^2\right]^{\frac{1}{2}} x$$

and when seeking the eigenvalue corresponding to m = 1 for example, with N = 8 and p = 1 say, a factor can be produced of size sinh 10x. At $x = \pi/2$ therefore, even though A_{2N-1} may be small, the solution could be affected by this factor. Clearly then the number of lines we use cannot be too large and it will be seen later that the N = 8 results are slightly affected by the instability while N = 7 results appear unaffected.

In the previous analytical solution of the MOL ordinary differential equations we obtained a solution explicitly involving x in the form sin px (p = 1,3, ...). Our choice of integration step length δx will now determine how accurately this factor is determined. Suppose we require the error in sin px to be less than 10^{-3} at $x = \pi/2$. The fourth order Runge Kutta and Hamming's predictor modifier corrector (Hamming, 1959) methods used in the computations yield errors

$$E < \left| \frac{\delta x^5}{120} f^{v}(\xi) \right|$$

on each step where $x < \xi < x + \delta x$ and f is the function of x being approximated. Integration from 0 to $\pi/2$ in n steps therefore gives a total error

$$E_T < n \left| \left[\frac{\pi}{2n}\right]^5 \frac{p^5}{120} \right|$$

from which follows $n > 3p^{5/4}$ or, for p = 5, $n > 24$. Since this is an upper bound on the error it was decided to use n = 20 steps from 0 to $\pi/2$ knowing then that this would produce sufficiently accurate results for p = 1,3 or 5.

It was decided to seek eigenvalues in the range $0 \leqslant k^2 \leqslant 65$ using N = 3,4,5, . . . as high as possible before inherent instability swamped the solution; this turned out to be N = 9. Since we expected a large number of eigenvalues in the above range and also some double and triple roots we selected an increment $\delta k^2 = 1$ to locate roughly the eigenvalues by the process mentioned earlier, see Equation (5.4). The resulting plots of $(\Sigma r_i^2)^{1/2}$ against k^2 are shown in Figure 5.1 where r_i is the residual in ψ_i' at $x = \pi/2$ after carrying out the minimization (5.2). The computation time for N = 3,4 . . . . 8 inclusive was 2 mins on an IBM 3032 computer.

The figures show that some roots are repeating for all values of N and therefore are reasonably accurate. Other roots however are not repeating and these are poor approximations to eigenvalues. For example, with N = 3, m = 5 and p = 1 we should have $k^2 = p^2 + m^2 = 26$ but obtain a root $k^2 \simeq 14.3$ which is consistent with values obtained in Table IXb. Having obtained these approximations we then locate the roots more accurately by minimization using Equation (5.5).

If we suspect double or triple roots, for example near $k^2 = 50$, we find one root in the usual manner and then minimize the function shown in (5.6).

Table IXc lists the values of k_{mp}^2 corresponding to (m,p) = (1,1) (3,3) (1,7) (7,1) and (5,5) obtained by this technique for N = 4,6,7 and 8. It can be seen that the values are consistent with those of Table IXb (add on p^2 to those values listed where p = 1,3,5,7).

The N = 8 solutions are affected by the inherent instability. This is demonstrated by Σr_i^2 being as large as 0.0015 when $k^2 = 2.0032$. The next eigenvalue k_{33}^2 is better than that predicted in Table IXb and therefore is likely to be a fortunate effect of the instability. The residuals in the (3,3) mode were much smaller than those of the (1,1) mode; this is caused by greater instability in the latter case.

The accuracy of the results can be seen to be very good for the (1,1) mode while for the higher modes the maximum error, excluding m = 7, is about 0.8%. The modes corresponding to m = 7 are not listed for $N < 8$ since they clearly are not very accurate even when N = 7 (Table IXb). The (1,7) mode is not as accurate as the (1,1) mode — greater accuracy for the (1,7) mode would require a smaller δx.

The local minimizations used to produce Table IXc took about one min. on an IBM 3032. Powell's (1964) one dimensional minimization was used.

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TABLE IXa

EIGENVALUES k^2-p^2 FOR THREE LINE SCHEME GIVEN BY FORMULA (5.12)

	m = 1	3	5	7
N = 3	0.9774	7.30	13.61	
4	0.9872	8.01	17.93	24.95
5	0.9918	8.35	20.26	32.18
6	0.9943	8.55	21.63	36.73
7	0.9958	8.67	22.48	39.72
8	0.9968	8.74	23.06	41.76
EXACT	1	9	25	49

TABLE IXb

EIGENVALUES k^2-p^2 FOR FIVE LINE SCHEME GIVEN IN FORMULA (5.16)

	m = 1	3	5	7	9	11
N = 3	1.0015	8.511	13.28			
4	1.0001	9.461	16.74	30.1		
5	1.0000	9.150	23.64	30.6	50.4	
6	1.0000	9.046	25.66	37.3	54.1	75
7	1.0000	9.014	25.42	46.3	56.5	83
8	1.0000	9.003	25.21	49.34	65.9	86
EXACT	1	9	25	49	81	121

TABLE IXc

NUMERICAL EVALUATION OF THE EIGENVALUES k^2_{mp} OF HELMHOLTZ' EQUATION IN A SQUARE OF SIDE π

	k^2_{11}	k^2_{33}	k^2_{17}	k^2_{71}	k^2_{55}
N = 4	2.0001	18.461	49.934		
6	2.0000	18.046	49.934		
7	2.0000	18.014	49.933		50.41
8	2.0032	18.001	49.940	50.34	50.20
EXACT	2	18	50	50	50

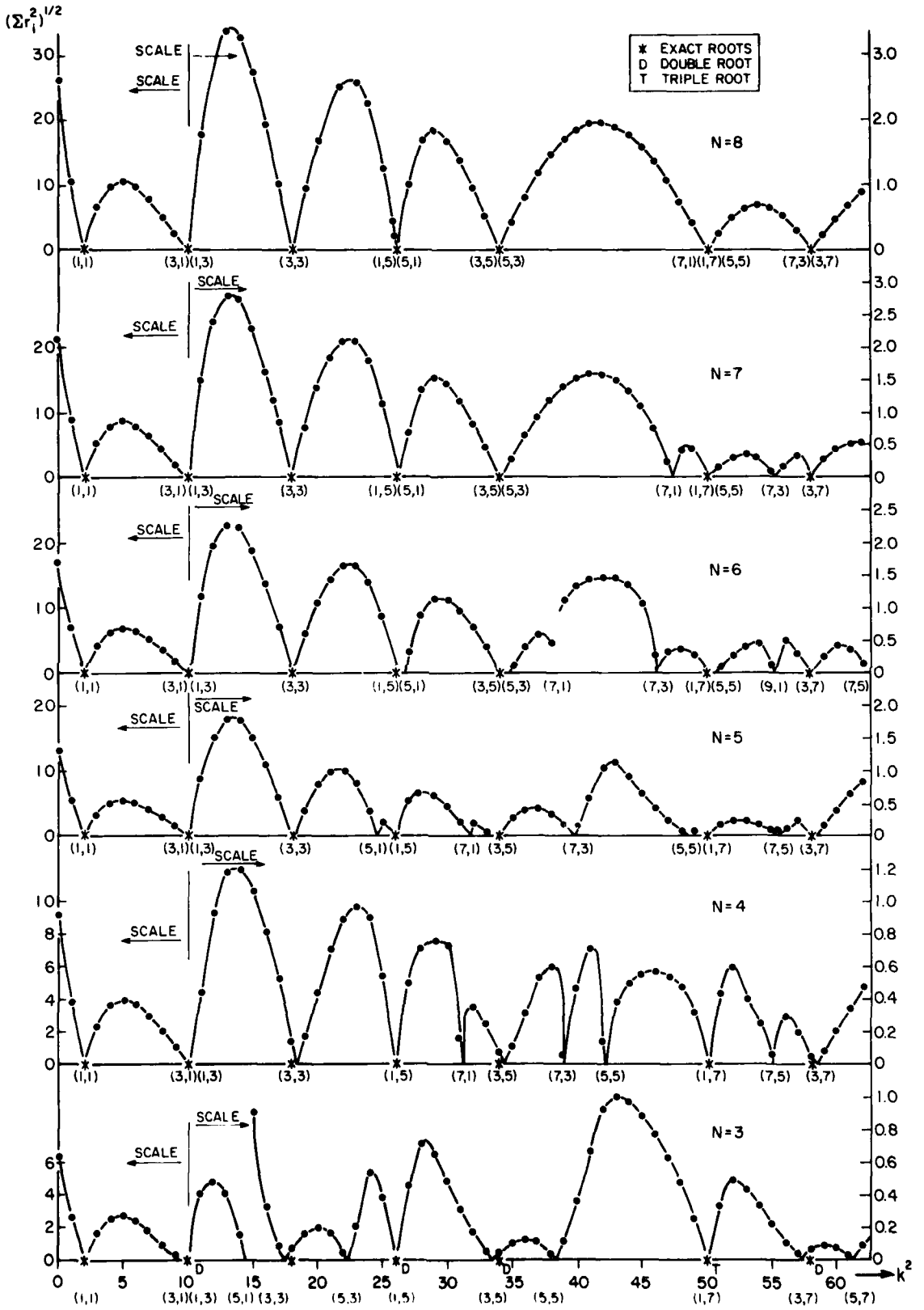

FIG. 5.1 RESIDUALS $(\Sigma r_i^2)^{1/2}$ vs. k^2 FOR SQUARE OF SIDE π. (m,p) ON k^2 AXIS REFERS TO EIGENVALUE k_{mp}^2 FROM TABLE IXb

APPENDIX A

The Method of Integral Relations

As mentioned in the Introduction, there is another semidiscrete method which has been widely used in aerodynamic problems, called the method of integral relations (MIR). Holt (1977) reviews the aerodynamic applications of the method, but theoretical treatments or studies of asymptotic convergence are rare.

The method is usually applied to systems of first-order partial differential equations. As in MOL, the region is considered to be divided into strips which are parallel to one co-ordinate, x say. The equations are partially integrated with respect to the other co-ordinate, y, to obtain an approximate system of ordinary differential equations. The partial integration is performed explicitly by assuming an appropriate y dependence of the integrands. Most applications have used for this purpose a polynomial whose degree increases proportionally to the number of strips. The algebraic development required for this procedure becomes very cumbersome for $N > 2$, so several investigators have used a linear y dependence from one line to the next in order to obtain a simple recursive form for a system of ordinary differential equations. We will consider the application of the latter procedure to the example of Section 3.3, since an explicit solution can then be found.

First the substitution $\psi_x = u$, $\psi_y = -v$ is made in Equation (3.4) to obtain the Cauchy-Riemann equations

$$u_x - v_y = 0; \qquad v_x + u_y = 0. \tag{A1}$$

With the polygon approximation for the y dependence, the partial integration with respect to y yields

$$\tfrac{1}{2}(u'_{n+1} + u'_n) - \frac{v_{n+1} - v_n}{h} = 0, \tag{A2}$$

$$\tfrac{1}{2}(v'_n + v'_{n+1}) + \frac{u_{n+1} - u_n}{h} = 0, \tag{A3}$$

where the notation is similar to that introduced in Equations (3.8) and (3.11). Differentiation of (A2) with respect to x and manipulation yields:

$$\tfrac{1}{4}(u''_{n+1} + 2u''_n + u''_{n-1}) + \frac{1}{h^2}(u_{n+1} - 2u_n + u_{n-1}) = 0, \tag{A4}$$

producing a tridiagonal system for the x derivatives.

The solution of the above system is in the identical form of Equations (3.20) and (3.22), except that

$$|\mu_m| = (2N/b)\tan(m\pi/4N), \tag{A5}$$

$$\cosh\theta = \left(1 + \frac{\pi^2 b^2}{4N^2}\right) \Big/ \left(1 - \frac{\pi^2 b^2}{4N^2}\right) \tag{A6}$$

From Equation (A5) we see that the largest eigenvalue is

$$\mu_{2N-1} \approx 8N^2/\pi b, \tag{A7}$$

giving Equation (3.25) for the instability factor in $\psi_n'(\frac{1}{2}) \equiv u_n(\frac{1}{2})$. Expansion of the hyperbolic cosine function as in Section 3.4 shows that the MIR discretization error is $0(N^{-2})$; but MIR is clearly inferior to MOL from the viewpoint of the size of the eigenvalues μ_m. That is, the MOL eigenvalues grow linearly with N, while the MIR eigenvalues are quadratic in N. Further, the extra complication of the tridiagonal system for the x derivatives has been added without gaining the benefit of decreased y-truncation error, contrary to the scheme of Appendix B.

APPENDIX B

Tridiagonal MOL Systems With Accuracy $0(N^{-4})$

As alternatives to the five-point difference schemes (2.17) we present here two schemes with the same accuracy $0(N^{-4})$ which involve only three adjacent lines. The schemes are not general but can be derived in certain cases as follows.

Poisson Equation

We have in the notation of this paper from Taylor-series expansions

$$\psi_{n+1} - 2\psi_n + \psi_{n-1} = h^2 \frac{\partial^2 \psi_n}{\partial y^2} + \frac{h^4}{12} \frac{\partial^4 \psi_n}{\partial y^4} + 0(h^6) \tag{B1}$$

and also

$$\frac{\partial^2 \psi_{n+1}}{\partial y^2} - 2 \frac{\partial^2 \psi_n}{\partial y^2} + \frac{\partial^2 \psi_{n-1}}{\partial y^2} = h^2 \frac{\partial^4 \psi_n}{\partial y^4} + 0(h^4). \tag{B2}$$

On eliminating $\partial^4 \psi_n / \partial y^4$ from (B1) and (B2) and substituting

$$\frac{\partial^2 \psi_k}{\partial y^2} = - \frac{\partial^2 \psi_k}{\partial x^2} + f(x, y_k) \qquad (k = n - 1, n, n + 1) \tag{B3}$$

from Poisson's equation, we obtain

$$\frac{1}{12}(\psi''_{n+1} + 10\psi''_n + \psi''_{n-1}) + h^{-2}(\psi_{n+1} - 2\psi_n + \psi_{n-1})$$

$$= \frac{1}{12}(f(x, y_{n+1}) + 10f(x, y_n) + f(x, y_{n-1})), \tag{B4}$$

giving a tridiagonal system of equations with accuracy $0(h^4)$ i.e., $0(N^{-4})$.

In fact the system (B4) can be solved analytically in certain cases and in particular we refer to the example of Section 3.3 and obtain the solution. It can be shown that this solution is identical to (3.20)-(3.22) except that

$$\mu_m = \frac{2N}{b} \sin\frac{m\pi}{4N} \cdot \left(1 - \frac{1}{3}\sin^2\frac{m\pi}{4N}\right)^{-1/2} \tag{B5}$$

and

$$\cosh\theta = \left(1 + \frac{5}{12}\frac{\pi^2 b^2}{N^2}\right) \Big/ \left(1 - \frac{\pi^2 b^2}{12N^2}\right) \tag{B6}$$

With this scheme the y-truncation error is reduced by two orders of magnitude compared to (2.5) while the largest eigenvalue μ_{2N-1} is increased only by a constant factor of about $\sqrt{(1.5)}$. We may expect to obtain results of accuracy comparable to the five-point scheme (2.17).

First-Order Equations

Consider the first-order equations

$$\frac{\partial P_i}{\partial x} + \frac{\partial Q_i}{\partial y} + R_i = 0 \tag{B7}$$

$i = 1, 2, \ldots, m$, where P_i, Q_i and R_i are linear or nonlinear functions of the independent and dependent variables, e.g., $P_i = P_i(x, y, u_1, u_2, \ldots, u_m)$. For instance the governing equations for two-dimensional flow can be written in the above form.

Dropping the i subscript and using Q_n to denote the value of Q on the n-th line for any one of the i values in Equation (B7) we have from Taylor-series expansions

$$\frac{Q_{n+1} - Q_{n-1}}{2h} = \frac{\partial Q_n}{\partial y} + \frac{h^2}{6}\frac{\partial^3 Q_n}{\partial y^3} + O(h^4) \tag{B8}$$

and also

$$\frac{\partial Q_{n+1}}{\partial y} - 2\frac{\partial Q_n}{\partial y} + \frac{\partial Q_{n-1}}{\partial y} = h\frac{\partial^3 Q_n}{\partial y^3} + O(h^4). \tag{B9}$$

Eliminating $\partial^3 Q_n/\partial y^3$ from (B8) and (B9) and substituting

$$(\partial Q_k/\partial y) = - R_k - (\partial P_k/\partial x) \qquad (k = n-1, n, n+1) \tag{B10}$$

gives

$$\frac{1}{6}(P'_{n+1} + 4P'_n + P'_{n-1}) + \frac{Q_{n+1} - Q_{n-1}}{2h} + \frac{1}{6}(R_{n+1} + 4R_n + R_{n-1}) = 0, \qquad \text{(B11)}$$

where $P'_k \equiv dP_k/dx$. Hence a tridiagonal system for the x derivatives is obtained which has error of order h^4, i.e., $0(N^{-4})$.

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